Lecture Notes

Parameter Identification

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Chapter 1

Introduction

The goal of this lecture is to provide an overview of important techniques used for the analysis, regularization, and numerical solution of *parameter identification problems*. Generally speaking, parameter identification problems deal with the reconstruction of unknown functions or geometric objects appearing as parameters (coefficients, right-hand sides, boundary values) in systems of differential equations. A parameter identification problem is a so-called *inverse problem*, in the sense that it somehow inverts the process of solving the differential equations.

A common property of a vast majority of inverse problems is their *ill-posedness*. In the sense of Hadamard, a mathematical problem (we can think of an equation or optimization problem) is well-posed if it satisfies the following properties:

1. **Existence:** For all (suitable) data, there exists a solution of the problem (in an appropriate sense).
2. **Uniqueness:** For all (suitable) data, the solution is unique.
3. **Stability:** The solution depends continuously on the data.

According to this definition, a problem is ill-posed if one of these three conditions is violated. However, in general we shall be concerned in particular with problems violating the third condition, i.e., the solution does not depend on the data in a stable way.

The prototype of an inverse problem will be an equation of the form

$$F(x) = y, \tag{1.1}$$

with a function space setting to be specified below. For such an equation, the unknown is x and the data are usually the right-hand side y. If the stability condition is violated, the numerical solution of the inverse problem by standard methods is difficult and often yields instability, even if the data are exact (since any numerical method has internal errors acting like noise). Therefore, special techniques, so-called *regularization methods* have to be used in order to obtain a stable approximation of the solution. Since the appropriate construction and analysis of regularization methods and subsequently (or simultaneously) of numerical schemes is the major issue in the solution of inverse problems, most of the lecture will be concerned with this task.

Inverse problems and parameter identification are very active fields of research in applied sciences, with a fast growing bibliography. Throughout the lecture notes we shall refer to

various papers and monographs including further details on several aspects. As general references on inverse problems, and also as sources for contents in this lecture we refer to the monographs by Engl, Hanke, Neubauer [13], Kirsch [18], and Vogel [24], the latter focusing on computational methods. As general literature on parameter identification we refer to the books by Banks and Kunisch [4], by Isakov [16, 17] and collections of papers in [3, 8, 15].

Chapter 2

Examples of Parameter Identification Problems

In the following we shall discuss some motivating examples of parameter identification problems. The first one, namely differentiation of data, is not a parameter identification problem in the strict sense, but is a good starting point to gain insight into properties of ill-posed problems. Moreover, it often appears as a subproblem in practical applications of parameter identification. We then proceed to a simple example of distributed parameter identification, which allows to discuss typical notions and properties of parameter identification problems. Finally, we give a short presentation of two prominent problems in parameter identification, namely electrical impedance tomography and inverse scattering, which rather serve as motivating examples than as sources for a detailed mathematical investigation at this stage.

2.1 Differentiation of Data

One of the simplest ill-posed problems is (numerical) differentiation of noisy functions, a task one faces in many applications. Assume that we want to compute the derivative of a function which includes additive noise, i.e., instead of the exact function f we are only given the function f^δ with

$$f^\delta(x) = f(x) + n^\delta(x), \qquad x \in [0,1]$$

and $f^\delta(0) = f(0) = 0$, $f^\delta(1) = f(1) = 0$, where $n^\delta(x)$ represents the data noise. In many typical measurement devices, the noise at each point x ($n^\delta(x)$) can be modeled as a normal distribution with mean zero and variance $\delta > 0$, being independent at different measurement points x_1 and x_2. From the law of large numbers one may expect that

$$\int_0^1 |n^\delta(x)|^2 \, dx \approx \delta^2,$$

i.e., one obtains some information of the noise. However, even if we know exactly that

$$\int_0^1 |n^\delta(x)|^2 \, dx = \delta^2$$

and δ is arbitrarily small, we cannot obtain any estimate on the derivative $\frac{df}{dx}$. In the worst case, the noise n^δ is not differentiable, so that one cannot even compute a derivative. However,

even if we assume that the noise is differentiable (even analytic) the error in the derivative can be arbitrarily large. Take for example

$$n^\delta(x) = \sqrt{2}\delta \sin(2\pi k x)$$

for some $k \in \mathbb{N}$. Then, $\int_0^1 |n^\delta(x)|^2 \, dx = \delta^2$ and

$$\frac{df^\delta}{dx}(x) = \frac{df}{dx}(x) + \sqrt{2}2\pi\delta k \sin(2k\pi x)$$

Now note that k can be arbitrarily large and therefore δk can be arbitrarily large. Hence, the L^2-error

$$\left(\int_0^1 \left(\frac{df^\delta}{dx}(x) - \frac{df}{dx}(x) \right)^2 \, dx \right)^{1/2} = 2\pi\delta k$$

or the L^∞-error

$$\sup_{x\in[0,1]} \left| \frac{df^\delta}{dx}(x) - \frac{df}{dx}(x) \right| = \sqrt{2}2\pi\delta k$$

can be arbitrarily large. This statement holds true in general for ill-posed problems (and could actually be used as a definition):

> *Without regularization and without further information, the error between the exact and noisy solution can be arbitrarily large, even if the noise is arbitrarily small.*

How can additional information that helps to bound the error, look like ? Of course, one could assume that the noise is bounded in a stronger norm, e.g.,

$$\int_0^1 \left(\frac{dn^\delta}{dx}(x) \right)^2 \, dx \leq \delta^2.$$

In this case, we would obtain in a trivial way the error estimate

$$\left(\int_0^1 \left(\frac{df^\delta}{dx}(x) - \frac{df}{dx}(x) \right)^2 \, dx \right)^{1/2} \leq \delta,$$

but our result does not correspond to the practical applications, where we can hardly get an estimate for $\frac{dn^\delta}{dx}$. Thus, it seems not a good idea to assume stronger bounds on the noise.

A more realistic alternative is to assume further regularity of the solution f, e.g., $f \in C^2([0,1])$. The error is then still arbitrarily large for the original problem, but can be estimated if regularization is used. As a simple example we could smooth the data by solving

$$-\alpha \frac{d^2 f_\alpha}{dx^2}(x) + f_\alpha(x) = f^\delta(x), \qquad f_\alpha(0) = f_\alpha(1) = 0,$$

which is also equivalent to applying the associated Green operator (an integral operator with smooth kernel) to f^δ. We shall see later that this approach can be identified with so-called *Tikhonov regularization*. Note that due to the standard variational interpretation of elliptic differential operators, this smoothing is also equivalent to mimimizing the functional

$$H_\alpha(f_\alpha) = \int_0^1 (f_\alpha(x) - f^\delta(x))^2 \, dx + \alpha \int_0^1 \left(\frac{df_\alpha}{dx}(x) \right)^2 \, dx,$$

i.e., we perform a least-squares fit with a penalty term that enforces $\frac{df_\alpha}{dx}$ to be bounded. Then we have

$$-\alpha\frac{d^2}{dx^2}(f_\alpha(x)-f(x))+(f_\alpha(x)-f(x))=(f^\delta(x)-f(x))+\alpha\frac{d^2f}{dx^2}(x)$$

and multiplication by $f_\alpha(x)-f(x)$ and integration with respect to x yields

$$\int_0^1\left[\alpha\left(\frac{df_\alpha}{dx}-\frac{df}{dx}\right)^2+(f_\alpha(x)-f(x))^2\right]dx=$$
$$\int_0^1\left(f^\delta(x)-f(x)+\alpha\frac{d^2f}{dx}\right)(f_\alpha(x)-f(x))\;dx$$

where we have used integration by parts for the first term. By applying the Cauchy-Schwarz inequality to the right-hand side we further obtain

$$\begin{aligned}\int_0^1\left[\alpha\left(\frac{df_\alpha}{dx}-\frac{df}{dx}\right)^2+\frac{1}{2}(f_\alpha(x)-f(x))^2\right]dx &\leq \int_0^1(f^\delta(x)-f(x))^2\;dx+\alpha^2C^2\\ &\leq \delta^2+\alpha^2C^2,\end{aligned}$$

where $C=\|f\|_{C^2}$. Thus, we may conclude in particular

$$\int_0^1\left(\frac{df_\alpha}{dx}-\frac{df}{dx}\right)^2dx\leq\frac{\delta^2}{\alpha}+\alpha C^2,$$

i.e., we obtain a bound on the error in terms of α and δ. The obvious next question is the choice of the regularization parameter: *How to choose α such that the error in the solution is minimal ?* In general it will not be possible to really minimize the error, but with an estimate like the one above we can at least minimize the right-hand side, which happens for $\alpha=\frac{\delta}{C}$ and the error estimate takes the form

$$\int_0^1\left(\frac{df_\alpha}{dx}-\frac{df}{dx}\right)^2dx\leq 2\delta.$$

If we take the square root in this estimat to obtain the norm on the left-hand side, the error is $\sqrt{2\delta}$, i.e., of order $\sqrt{\delta}$ and hence, much larger than the data error δ. This is another typical effect for ill-posed problems: *Even with regularization, we can never achieve an error in the reconstruction which is as slow as the error in the data.* Note also that the error bound $\sqrt{2\delta}$ was only achieved for $f\in C^2([0,1])$. If we only assume that $f\in C^1([0,1])$, which seems actually much more natural for differentiating once, we would need to estimate alternatively

$$\begin{aligned}\int_0^1\alpha\frac{d^2f}{dx}(f_\alpha(x)-f(x))\;dx &= -\alpha\int_0^1\alpha\frac{df}{dx}(\frac{df_\alpha}{dx}(x)-\frac{df}{dx}(x))\;dx\\ &\leq \frac{\alpha}{2}\int_0^1\left(\frac{df_\alpha}{dx}-\frac{df}{dx}\right)^2dx+\frac{\alpha}{2}\int_0^1\left(\frac{df}{dx}\right)^2dx.\end{aligned}$$

Since the second integral can be estimated by $\frac{\alpha}{2}C^2$ with $C=\|f\|_{C^1}$ the final estimate becomes

$$\int_0^1\left(\frac{df_\alpha}{dx}-\frac{df}{dx}\right)^2dx\leq 2\frac{\delta^2}{\alpha}+C^2,$$

and the right-hand side is larger than C no matter how we choose α. As we shall see later, one can show by different arguments that $\int_0^1 \left(\frac{df_\alpha}{dx} - \frac{df}{dx}\right)^2 \, dx \to 0$, but this convergence is arbitrarily slow, another general statement for ill-posed problems: *Without additional smoothness assumptions on the exact solution, the convergence of regularized solutions is arbitrarily small.*

Above we have motivated inverse problems as the inversion of some kind of direct problem. For numerical differentiation, we have started with the inverse problem immediately. However, the direct problem can easily be obtained by integration. E.g., if $f(0) = 0$, then the direct problem is given by the integral equation of the first kind

$$f^\delta(x) = \int_0^x \frac{df}{dx}(y) \, dy.$$

This integral operator can be shown to be compact and we will see later that the inversion of a compact linear operator is always an ill-posed problem.

We finally mention that analogous reasoning can be applied to numerical differentiation of sampled data of a function f, e.g. by one-sided or central finite difference schemes. In this case, the difference scheme has the effect of a regularization method and the grid size h plays the role of a regularization parameter. A detailed analysis can be found in [13, 20].

2.2 Parameter Identification with Distributed Data

By parameter identification one usually denotes the problem of reconstructing unknown coefficients in partial differential equations from indirect measurements of the solution. A simple example is the following model from *groundwater filtration*, which is modeled through the elliptic equation

$$-\text{div } (a\nabla u) = f, \qquad \text{in } \Omega \subset \mathbb{R}^d,$$

where u is the unkown, f a given source, and a the hydraulic permittivity. The direct problem consists in solving the partial differential equation for u given a and suitable boundary conditions on $\partial\Omega$. The inverse problem consists in reconstructing the unknown function a on Ω given a noisy measurement

$$u^\delta(x) = u(x) + n^\delta(x), \qquad x \in \Omega,$$

of the solution.

If the solution of the direct problem is unique for each parameter a, which is the case for the groundwater filtration problem with appropriate boundary conditions, then one can introduce the *parameter-to-solution map* $a \mapsto u_a$, where u_a is the solution of the direct problem given a specific a. Note that even if the direct problem is linear (for u), the inverse problem and the parameter-to-output map are usually nonlinear. E.g., in the groundwater filtration problem we have $u_{2a} = \frac{1}{2}u_a$, i.e., $u_{2a} \neq 2u_a$ and hence, the problem is not linear.

The uniqueness question for parameter identification problems is usually denoted as *identifiability*. In the case $\Omega = [0, 1]$ with boundary conditions $\frac{du}{dx}(0) = 0$ and $u(1) = 0$ we can easily answer the question by integrating the equation with respect to x, which yields the formula

$$a(x)\frac{du}{dx}(x) = \int_0^x f(y) \, dy.$$

Hence, the parameter a is determined uniquely for every x such that $\frac{du}{dx}(x) \neq 0$. On the other hand, there are many realistic assumptions on f, which guarantee that $\frac{du}{dx} \neq 0$ almost everywhere. For example, if the antiderivative of f is positive in $(0,1)$, then the above formula shows that $\frac{du}{dx} \neq 0$. Another possible assumption is $f(x) \neq 0$ for almost every x, then $\frac{du}{dx}$ cannot vanish on an open interval $I \subset [0,1]$, since otherwise

$$0 = \frac{d0}{dx} = \frac{d}{dx}\left(a(x)\frac{du}{dx}(x)\right) = f(x), \qquad x \in I$$

yields a contradiction. On the other hand, if $f \equiv 0$, then $u \equiv 0$ and $\frac{du}{dx} \equiv 0$ for any a and it is never possible to reconstruct the parameter. The choice of f or in reality the action leading to the source f is a matter of *design of experiments*, one could even ask the question what is the best source with respect to stable reconstruction of the parameter.

The solution formula

$$a(x) = \frac{\int_0^x f(y)\ dy}{\frac{du}{dx}(x)}$$

also shows that besides the usual *linear ill-posedness* arising from the fact that data (u) have to be differentiated, there is a *nonlinear ill-posedness* from the quotient, whose consequence is that errors at small values of $\frac{du}{dx}$ are amplified much stronger than errors at large values of $\frac{du}{dx}$. I.e., if $\frac{du}{dx}(x)$ is very small in an interval I, then we still have identifiability, but in practice we must expect very high errors due to the noise amplification.

Another interesting issue in parameter identification problems are stability estimates, which concerns the continuity of the inverse operator on special subsets. Note that for an ill-posed problem, the inverse operator (if it exists) is not continuous, but it is continuous on compact subsets of its domain. As an example we consider the compact subset

$$\mathcal{C}_{\gamma,M} = \{\ u \in C^2([0,1])\ |\ , \|u\|_{C^2} \leq M, \frac{du}{dx} \geq \gamma > 0 \text{ in } [0,1]\ \}.$$

Let u_j be the solution of the forward problem for given parameter a_j, $j = 1, 2$. Then, from the above inversion formula we obtain

$$a_1(x) - a_2(x) = \frac{\int_0^x f(y)\ dy}{\frac{du_1}{dx}(x)\frac{du_2}{dx}(x)}\left(\frac{du_2}{dx}(x) - \frac{du_1}{dx}(x)\right)$$

Hence, we obtain

$$\int_0^1 (a_1(x) - a_2(x))^2\ dx \leq \frac{(\int_0^1 |f(y)|\ dy)^2}{\gamma^4}\int_0^1 \left(\frac{du_2}{dx}(x) - \frac{du_1}{dx}(x)\right)^2\ dx.$$

Using integration by parts and the Cauchy-Schwarz inequality we obtain

$$\begin{aligned}
&\int_0^1 \left(\frac{du_2}{dx}(x) - \frac{du_1}{dx}(x)\right)^2\ dx \\
&\quad = \int_0^1 (u_1(x) - u_2(x))\left(\frac{d^2u_2}{dx}^2(x) - \frac{d^2u_1}{dx}^2(x)\right)\ dx \\
&\quad \leq \sqrt{\int_0^1 (u_1(x) - u_2(x))^2\ dx}\sqrt{\int_0^1 \left(\frac{d^2u_2}{dx^2}(x) - \frac{d^2u_1}{dx^2}(x)\right)^2\ dx} \\
&\quad \leq 2M\|u_1 - u_2\|_{L^2}
\end{aligned}$$

Thus, for the difference $a_1 - a_2$ we obtain the estimate

$$\|a_1 - a_2\|_{L^2} \leq \frac{\|f\|_{L^1}}{\gamma^2}\sqrt{2M}\|u_1 - u_2\|_{L^2}^{1/2},$$

i.e., the inverse operator $G : u \in \mathcal{C}_\gamma \mapsto a$ is locally Hölder continuous with exponent $\frac{1}{2}$ in the L^2-norm. This result corresponds to the Hölder estimate we have derived for numerical differentiation above. The effect that the estimate is only a local one for the parameter identification problem, is a consequence of the nonlinearity. One clearly observes the influence of smoothness of the solution, for increasing M the constant in the Hölder estimate increases. Moreover, the nonlinear instability is reflected in the estimate by the term $\frac{1}{\gamma^2}$, i.e., the closer u gets to zero, the larger the constant becomes.

In practical applications, it is hardly the case that the solution of a partial differential equation can be measured on a whole domain, since one usually cannot place many detectors inside an object (e.g. a patient in medical applications or a microelectronic device). In such cases boundary measurements either on a space- or time-boundary are available. An example is the diffusion equation

$$\frac{\partial u}{\partial t} = \text{div } (a\nabla u) + f \qquad \text{in } \Omega \times (0, T),$$

with measurements at final time, i.e., $u(x, T)$, for $x \in \Omega$, or at the boundary, e.g., $\frac{\partial u}{\partial n}$ on $\partial\Omega \times (0, T)$. Of course, with such a measurement, the dimensionality of the data is much lower than the one of the unknown $a(x, t)$. Thus, in such cases one can only identify special parameters such as $a = a(x)$, which is however realistic since a might describe material properties that do not change in time.

2.3 Impedance Tomography

Impedance tomography can be considered as a parameter identification problem with boundary measurements. The technological setup is as follows: at the boundary of an object (represented by a domain $D \subset \mathbb{R}^d$), different electrical voltages are applied, and the arising electrical currents are measured. From these measurements one would like to reconstruct the conductivity as a function of space, which gives information about different materials inside the object.

The simplest mathematical model for this process is the solution of the elliptic partial differential equation

$$\text{div } (a\nabla u) = 0 \qquad \text{in } D,$$

where u is the electric potential and a is the conductivity, modeled as a function of the spatial location inside D. The applied voltages f are directly related to the electric potential u at the boundary, i.e.,

$$u = f \qquad \text{on } \partial D.$$

The measured currents over the boundary for a specific voltage f are given by

$$g_f = a\frac{\partial u}{\partial n} \qquad \text{on } \partial D.$$

Hence, if all possible voltages f (in the sense of all functions on ∂D in a certain class) are applied, and the corresponding currents are measured, the data consist of the *Dirichlet-to-Neumann map*

$$\Lambda_a : f \mapsto g_f,$$

which is a linear operator due to the linearity of the differential equation and boundary conditions for fixed a.

The inverse problem of impedance tomography (called *inverse conductivity problem*) consists in reconstructing the conductivity a as a function on D from a measurement of the Dirichlet-to-Neumann map Λ_a. Again, due to the appearance of a as a coefficient in the equation, the inverse problem is nonlinear, though the direct problem of computing the Dirichlet-Neumann map for given a is linear.

From the dimensionality of the data it is not clear whether one can reconstruct the conductivity uniquely, since the unknown is a function on D and the measurement is a linear operator on a class of functions on ∂D. The answer depends on the spatial dimension, for $d \geq 2$ it is indeed possible to identify the conductivity uniquely if the class of voltages f on ∂D is sufficiently large. For dimension $d = 1$, the answer is negative. Consider e.g. the domain $D = [0, 1]$ with boundary $\partial D = \{0, 1\}$. Then a function f on ∂D can be represented by two values, f_0 for $x = 0$, and f_1 for $x = 1$. Hence, the Dirichlet-to-Neumann map can be considered as a linear operator $\Lambda_a : \mathbb{R}^2 \to \mathbb{R}^2$. Since each such linear operator can be represented by a 2×2 matrix, the data consist only of 4 real numbers representing the matrix entries, Since the dimension of the data space ($\mathbb{R}^{2\times 2}$) is finite, but the dimension of the space for the unknown (e.g. $C^1(D)$) is infinite, the data cannot suffice to determine the conductivity uniquely.

An interesting case in impedance tomography is the case of objects consisting only of two different materials and consequently of two different conductivity values, i.e.,

$$a(x) = \begin{cases} a_1 & \text{if } x \in \Omega \subset D \\ a_2 & \text{if } x \in D \backslash \Omega. \end{cases}$$

The subset Ω could for example represent the shape of some inclusion in the object. In such a case the interest is focused on identifying the shape Ω. Since the class of possible functions a is now strongly limited by introducing a-priori knowledge, one may argue that less measurements suffice in order to obtain uniqueness, at least for the shape Ω at given values a_1 and a_2. Indeed, one can show that the measurement of the Neumann value for a single Dirichlet value yields local uniqueness of the inverse problem.

2.4 Inverse Scattering

Inverse scattering problems are, generally speaking, inverse problems where one tries to recover information about an unknown object from measurements of waves (or fields) scattered by this object. Inverse scattering problems exist for all kinds of waves (e.g. acoustic and electromagnetic waves) and all kinds of models (e.g. wave equation, Helmholtz equation, Schrödinger equation, Maxwell equations). We consider the case of an acoustic scattering problem for the Helmholtz equation in the following.

The original mathematical model for the density of an acoustic wave is the wave equation

$$\frac{\partial^2 U}{\partial t} = \frac{1}{n^2} \Delta u \qquad \text{in } \mathbb{R}^d \times \mathbb{R}_+,$$

where $n = n(x)$ describes a spatially varying *acoustic profile* (reciprocal to the speed of sound), where n is scaled to equal one outside a compact domain ($n = 1$ may e.g. represent surrounding air or water). The region where $n(x) \neq 1$ represents the *scattering object*, the deviation of $n(x)$ from one provides information about the structure of the scatterer. If we only consider time harmonic waves of the form $U(x,t) = e^{ikt}u(x)$ for $k \in \mathbb{R}$, then the function u solves the Helmholtz equation

$$\Delta u + k^2 n^2 u = 0.$$

In inverse scattering, an incident wave u^i is sent in, which corresponds to the wave propagating in absence of the scatterer, i.e.,

$$\Delta u^i + k^2 u^i = 0.$$

The scattered wave, which is the difference between the really observed and the incident wave, i.e., with $u^s = u - u^i$ satisfies

$$\Delta u^s + k^2 u^s = k^2 f(u^i + u^s),$$

$f := 1 - n^2$. The inverse scattering problem consists in identifying the compactly supported function f from the knowledge of the incident wave u^i and a measurement of the scattered wave u^s. The scattered wave can only be measured far away from the scatterer, in many cases it is reasonable to assume that u^s can be measured at the sphere with radius $R >> 1$ including the scatterer, which is referred to as the *far-field pattern*.

A closer look at the dimensonality of the unknown (f) and the data ($u^s|_{r=R}$) shows that we have to identify a function on a d-dimensional domain ($d = 2, 3$), but the measurement is a function on a $d-1$-dimensional manifold. Hence, it seems obvious that a single measurement will not suffice to determine f uniquely. For this reason, one uses many different incident waves (varying the value of k) and measures the far-field pattern for all of them, which yields reasonable data for the inverse problem.

Due to the appearance of f as a coefficient in the Helmholtz equation, the acoustic inverse scattering problem is nonlinear. In several situations it is reasonable to assume that the scattered wave in a neighborhood of the scatterer is much smaller than the incident wave, i.e., the term $u^i + u^s$ on the right-hand side can be approximated well by u^i. Under this assumption one can use a linearized version of the inverse scattering problem via the equation

$$\Delta u^s + k^2 u^s = k^2 f u^i,$$

which is known as the *Born approximation*.

A related situation is *inverse obstacle scattering*, where the scattering appears at an obstacle (represented by a domain D), which is not penetrated by the wave. In this case, the Helmholtz equation is a model for wave propagation outside D, i.e.,

$$\Delta u + k^2 u = 0 \qquad \text{in } \mathbb{R}^d \backslash D,$$

coupled with a boundary condition of the form

$$\frac{\partial u}{\partial n} + \lambda u = 0 \qquad \text{on } \partial D.$$

The inverse obstacle scattering problem consists in identifying the shape D, and similary to the corresponding situation for electrical impedance tomography this can be achieved using less measurements (i.e., for only few values of k).

Chapter 3

Tikhonov-type Regularization

In this section we investigate Tikhonov regularization and related schemes more closely. In general, we shall now consider a nonlinear operator equation of the form

$$F(x) = y, \tag{3.1}$$

where $F : X \to Y$ is a continuous nonlinear operator. The extension of the regularization method to the nonlinear case is not obvious, since one can neither carry out a singular value decomposition nor define an adjoint of a nonlinear operator. The generalization to the nonlinear case therefore needs a reformulation of Tikhonov regularization, which we shall discuss in the following.

3.1 Tikhonov Regularization

We start from the Tikhonov regularization of a linear operator equation, which is determined by the solution of the equation

$$(A^*A + \alpha I)x_\alpha^\delta = A^*y^\delta.$$

It is easy to verify that this linear equation is the first order optimality condition of the quadratic optimization problem

$$J_\alpha(x) := \|Ax - y^\delta\|^2 + \alpha\|x\|^2 \to \min_{x\in X}. \tag{3.2}$$

Note thatJ_α is strictly convex, which follows from

$$J''(x)(\varphi,\varphi) = 2\|A\varphi\|^2 + 2\alpha\|\varphi\|^2 > 0$$

and hence, x_α^δ is the unique global minimizer of the functional J_α.

The characterization of the regularized solution as a minimizer of the functional (3.2) offers the possibility of an immediate generalization to the nonlinear case, since we can define a regularized solution via

$$x_\alpha^\delta \in \arg\min_{x\in X}\left[\|F(x) - y^\delta\|^2 + \alpha\|x - x^*\|^2\right]. \tag{3.3}$$

Here, $x^* \in X$ is a given prior, which might represent a-priori knowledge about the solution. Note that in the nonlinear case, the value $x^* = 0$ plays no special role, so we can in principle consider any prior x^*. Consequently, we must also adapt our definition of generalization solution to the nonlinear case:

Definition 3.1. We shall call $\overline{x} \in X$ *least-squares solution* of (3.1) if

$$\|F(\overline{x}) - y\| = \inf_{x \in X} \|F(x) - y\|.$$

A least-squares solution $x^\dagger$ is called x^*-minimum norm solution, if

$$\|x^\dagger - x^*\| = \inf\{ \|x - x^*\| \mid x \text{ is least squares solution of (3.1)} \}.$$

For general nonlinear operators, we cannot expect the functional

$$J_\alpha(x) := \|F(x) - y^\delta\|^2 + \alpha\|x - x^*\|^2 \tag{3.4}$$

to be convex and hence, minimizers need not be unique. Moreover, there may exist global as well as local minimizers, but we will only consider global minimizers as regularized solutions.

We start with differentiability properties of the functional J_α:

Proposition 3.2. *If F is Frechet-differentiable, then the functional $J_\alpha : X \to \mathbb{R}$ is is Frechet-differentiable with derivative*

$$J'_\alpha(x)\varphi = 2\langle F(x) - y, F'(x)\varphi\rangle + 2\alpha\langle x - x^*, \varphi\rangle. \tag{3.5}$$

Moreover, irf F is twice Frechet-differentiable, then the functional $J_\alpha : X \to \mathbb{R}$ is is Frechet-differentiable with second derivative

$$J''_\alpha(x)(\varphi_1, \varphi_2) = 2\langle F'(x)\varphi_1, F'(x)\varphi_2\rangle + 2\langle F(x) - y, F''(x)(\varphi_1, \varphi_2)\rangle + 2\alpha\langle\varphi_1, \varphi_2\rangle. \tag{3.6}$$

Again, we can use the first-order optimality condition to verify that a regularized solution satisfies

$$F'(x_\alpha^\delta)^*(F(x_\alpha^\delta) - y^\delta) + \alpha(x_\alpha^\delta - x^*) = 0, \tag{3.7}$$

the nonlinear analogue of the original equation. On the other hand, not every solution of (3.7) is necessarily a regularized solution, since it could as well be a local minimum, saddle-point, or even maximum of J_α.

So far, we have not yet considered the problem of existence of regularized solutions, which is not obvious in the nonlinear case. In order to prove existence, we need an additional condition, namely *weak sequential closedness* of the operator F:

$$F(x) = y \qquad \text{if } F(x_n) \rightharpoonup y, x_n \rightharpoonup x. \tag{3.8}$$

This assumption is no severe restriction for inverse problems, in particular every compact nonlinear operator is weakly sequentially closed.

Theorem 3.3. *Let $F : X \to Y$ be a continuous operator satisfying* (3.8)*. Then, there exists a minimizer $x_\alpha^\delta \in X$ of the functional J_α defined by* (3.4)*.*

Proof. We first consider the level sets $L_M := \{ x \in X \mid J_\alpha(x) \le M \}$. Since $J_\alpha(x^*) = \|F(x^*) - y^\delta\|^2 < \infty$, the set L_M is nonempty for M sufficiently large. Moreover, $x \in L_M$ implies $\alpha\|x - x^*\|^2 \le M$ and, due to the triangle inequality

$$\|x\| \le \|x_*\| + \sqrt{\frac{M}{\alpha}} =: R,$$

i.e., L_M is contained in a ball with radius R. Since balls in X are compact with respect to the weak topology, the sets L_M are weakly pre-compact.

Since J_α is bounded below by zero, its infimum is finite and thus, there exists a minimizing sequence x_n. Since $x_n \in L_M$ for n sufficiently large, we can extract a weakly convergent subsequence (again denoted by x_n) with some limit $\overline{x} \in X$. Moreover, the sequence $F(x_n)$ is bounded due to

$$\|F(x_n) - y^\delta\|^2 \leq M$$

and hence, there exists a weakly convergent subsequence (again denoted by the subscript n) $F(x_n) \rightarrow z \in Y$. Because of the weak sequential closedness, we conclude $z = F(\overline{x})$, and thus,

$$J_\alpha(\overline{x}) = \lim_{n\to\infty} J_\alpha(x_n) = \inf_{x\in X} J_\alpha(x),$$

i.e. $x_\alpha^\delta = \overline{x}$ is a minimizer of J_α. □

We now turn our attention to the stability properties of Tikhonov regularization for (3.1). In the linear case, we have derived a Lipschitz estimate for the regularization operators, which is not possible in the general nonlinear case. In the nonlinear case, we only obtain a weak stability in a set-valued sense:

Proposition 3.4. *Let $F : X \rightarrow Y$ be a continuous operator satisfying* (3.8)*. Moreover, let $y_n \in Y$ be a sequence such that $y_n \rightarrow y^\delta$ and let x_n be a corresponding sequence of minimizers of J_α with y^δ replaced by y_n. Then x_n has a weakly convergent subsequence and every weak accumulation point is a minimizer of J_α.*

Proof. Due to Theorem 3.3 we can find a sequence of minimizers x_n corresponding to the data y_n. Since

$$\|x_n - x_*^2\| \leq \frac{1}{\alpha}\|F(x_n) - y_n\|^2 + \|x_n - x^*\|^2 \leq \frac{1}{\alpha}\|F(x^*) - y_n\|^2$$

and since y_n converges to y^δ, x_n is contained in a ball with radius independent of n. Due to weak compactness we can extract a convergent subsequence. Now let x be a weak accumulation point of x_n, without restriction of generality we assume that $x_n \rightharpoonup x$. Since $\|F(x_n) - y_n\| \leq \|F(x^*) - y_n\|$ we also conclude boundedness of $F(x_n)$ and consequently existence of a weak subsequence with limit z, and the weak sequential closedness implies $z = F(x)$. Finally, from the weak lower semicontinuity of the square of the norm in Hilbert spaces we conclude

$$\begin{aligned} J_\alpha(x) &= \|F(x) - y^\delta\|^2 + \alpha\|x - x^*\|^2 \leq \liminf_n \|F(x_n) - y_n\|^2 + \alpha\|x_n - x^*\|^2 \\ &\leq \liminf_n \|F(x_\alpha^\delta) - y_n\|^2 + \alpha\|x_\alpha^\delta - x^*\|^2 \\ &= \|F(x_\alpha^\delta) - y_\delta\|^2 + \alpha\|x_\alpha^\delta - x^*\|^2 = J_\alpha(x_\alpha^\delta). \end{aligned}$$

Since x_α^δ is a minimizer of J_α, x must be a minimizer, too. □

Proposition 3.4 ensures that Tikhonov regularization has indeed a regularizing effect, i.e., the approximate problems are well-posed for $\alpha > 0$. The obvious next question is convergence of the regularization method with suitable choice of α in dependence on δ. As for stability, this convergence apppears in a set-valued sense:

Theorem 3.5. *Let $y \in Y$ such that there exists a x^*-minimum norm solution $x^\dagger \in X$ with $F(x^\dagger) = y$. Let y^δ be noisy data satisfying*

$$\|y - y^\delta\| \leq \delta$$

and let x_α^δ be a regularized solution satisfying (3.3). If $\alpha = \alpha(\delta, y^\delta)$ is chosen such that

$$\alpha \to 0, \qquad \frac{\delta^2}{\alpha} \to 0 \qquad \text{as } \delta \to 0, \tag{3.9}$$

then there exists a strongly convergent subsequence $x_{\alpha_n}^{\delta_n}$ (with $\delta_n \to 0$) and the limit of each convergent subsequence is a x^*-minimum norm solution of (3.1).

Proof. Since x_α^δ is a minimizer of J_α, we conclude

$$\begin{aligned} \|x_\alpha^\delta - x^*\|^2 &\leq \frac{1}{\alpha}\|F(x_\alpha^\delta) - y^\delta\|^2 + \|x_\alpha^\delta - x^*\|^2 = \frac{1}{\alpha} J_\alpha(x_\alpha^\delta) \\ &\leq \frac{1}{\alpha} J_\alpha(\overline{x}) = \frac{1}{\alpha}\|F(x^\dagger) - y^\delta\|^2 + \|x^\dagger - x^*\|^2 \\ &\leq \frac{\delta^2}{\alpha} + \|x^\dagger - x^*\|^2. \end{aligned}$$

Since $\frac{\delta^2}{\alpha} \to 0$, it is bounded in particular, and hence, $\|x_\alpha^\delta - x^*\|$ is uniformly bounded with respect to δ, which allows to extract a weakly convergent subsequence. For $x_{\alpha_n}^{\delta_n}$ being a weakly convergent subsequence with limit $\overline{x}$, the above estimate yields

$$\|\overline{x} - x^*\|^2 \leq \limsup_n \|x_{\alpha_n}^{\delta_n} - x^*\|^2 \leq \limsup_n \frac{\delta_n^2}{\alpha_n} + \|x^\dagger - x^*\|^2 = \|x^\dagger - x^*\|^2$$

and

$$\|F(\overline{x} - y\|^2 \leq \limsup_n \|F(x_{\alpha_n}^{\delta_n}) - y^\delta\|^2 \leq \limsup_n (\delta_n^2 + \alpha_n \|x^\dagger - x^*\|^2) = 0.$$

Hence, $\overline{x}$ satisfies $F(\overline{x}) = y$ and, by the definition of the least-squares solution

$$\|\overline{x} - x^*\| \leq \|x^\dagger - x^*\| = \inf\{\ \|x - x^*\| \mid x \text{ is least squares solution of (3.1)}\ \},$$

which implies that $\overline{x}$ is a least-squares solution of (3.1).

It remains to verify strong convergence of $x_{\alpha_n}^{\delta_n}$. For this sake we expand

$$\|x_{\alpha_n}^{\delta_n} - \overline{x}\|^2 = \|x_{\alpha_n}^{\delta_n} - x^*\|^2 + \|\overline{x} - x^*\|^2 - 2\langle x_{\alpha_n}^{\delta_n} - x^*, \overline{x} - x^*\rangle.$$

Due to the weak convergence we know that

$$-2\langle x_{\alpha_n}^{\delta_n} - x^*, \overline{x} - x^*\rangle \to -2\|\overline{x} - x^*\|^2.$$

Moreover, we have concluded above that

$$\limsup_n \|x_{\alpha_n}^{\delta_n} - x^*\|^2 \leq \|\overline{x} - x^*\|^2,$$

and thus,

$$\limsup_n \|x_{\alpha_n}^{\delta_n} - \overline{x}\|^2 \leq \|\overline{x} - x^*\|^2 + \|\overline{x} - x^*\|^2 - 2\|\overline{x} - x^*\|^2 = 0,$$

which implies the strong convergence. □

Note that the convergence prove applies only to situations where the data y are attainable, i.e., $F(x^\dagger) = y$. If $\|F(x^\dagger) - y\| > 0$ a slightly different proof under changed conditions on the parameter choice has to be carried out, we refer to [5] for further details.

We finally consider convergence rates in the nonlinear setting. For the sake of simplicity we restrict our attention to the case corresponding to $\mu = \frac{1}{2}$ for the linear problem. In this case, the source condition $x^\dagger = (A^*A)^{(1/2)}w$ is equivalent to $x^\dagger = A^*p$ for

$$p = \sum_{n=1}^{\infty} \langle w, u_n \rangle v_n \quad \in Y.$$

The condition $x^\dagger = A^*p$ is easier to interpret from an optimization point of view. A mininum norm solution $x^\dagger$ is determined as a minimizer of the constrained problem

$$\frac{1}{2}\|x\|^2 \to \min_{x \in X}, \text{ subject to } Ax = y,$$

and it is natural to consider the associated Lagrangian

$$L(x; p) := \frac{1}{2}\|x\|^2 - \langle Ax, y \rangle.$$

It is easy to see that for $(x^\dagger, p)$ being a stationary point of the Lagrangian, $x^\dagger$ is a solution of the above constrained problem, i.e., a minimum norm solution. In the case of an ill-posed operator equation, the converse does not hold, since the constraint operator A^* is not surjective. Hence, the existence of a Lagrange multiplier is an additional smoothness condition on the exact solution $x^\dagger$. Since we always have $\frac{\partial}{\partial p}L(x^\dagger; p) = Ax^\dagger - y = 0$, it is clear that a stationary point p exists if and only if

$$0 = \frac{\partial}{\partial x}L(x^\dagger; p) = x - A^*p,$$

i.e., if and only if the source condition is satisfied.

Again, the optimization viewpoint allows an immediate generalization to the nonlinear case, where the Lagrangian is given by

$$L(x; p) = \frac{1}{2}\|x - x^*\|^2 \langle F(x) - y, p \rangle.$$

Thus, the source condition becomes

$$0 = \frac{\partial}{\partial x}L(x^\dagger; p) = x^\dagger - x^* - F'(x^\dagger)^*p,$$

i.e.,

$$\exists\, p \in Y : \quad x^\dagger - x^* = F'(x^\dagger)^*p. \tag{3.10}$$

In order to prove a convergence rate we also assume that F' is Lipschitz continuous with module L and that the smallness condition

$$L\|p\| < 1 \tag{3.11}$$

holds.

Theorem 3.6. *In addition to the assumptions of Theorem 3.5 assume that* (3.10) *and* (3.11) *hold. Moreover, if* $\alpha(\delta, y^\delta) \sim \delta$*, there exists* $\delta_0 > 0$*, such that for all* $\delta < \delta_0$ *the estimate*

$$\|x_\alpha^\delta - x^\dagger\| \leq c\sqrt{\delta} \tag{3.12}$$

holds for some constant $c > 0$*.*

Proof. Since x_α^δ minimizes J_α we obtain

$$\|F(x_\alpha^\delta) - y^\delta)\|^2 + \alpha\|x_\alpha^\delta - x^*\|^2 \leq \delta^2 + \alpha\|x^\dagger - x^*\|^2$$

and after a simple calculation, this inequality can be rewritten as

$$\|F(x_\alpha^\delta) - y^\delta)\|^2 + \alpha\|x_\alpha^\delta - x^\dagger\|^2 \leq \delta^2 + 2\alpha\langle x^\dagger - x^*, x^\dagger - x_\alpha^\delta\rangle. \tag{3.13}$$

Now we insert the source condition (3.10) into the last term on the right-hand side to obtain

$$-2\alpha\langle x^\dagger - x^*, x^\dagger - x_\alpha^\delta\rangle = 2\alpha\langle p, F'(x^\dagger)(x_\alpha^\delta - x^\dagger)\rangle.$$

From a Taylor-expansion we obtain that

$$F'(x^\dagger)(x_\alpha^\delta - x^\dagger)\rangle = F(x_\alpha^\delta) - F(x^\dagger) + r_\alpha^\delta,$$

and due to the Lipschitz continuity of F' we have

$$\|r_\alpha^\delta\| \leq \frac{L}{2}\|x_\alpha^\delta - x^\dagger\|^2.$$

Hence, we may estimate

$$2\alpha\|\langle p, F'(x^\dagger)(x_\alpha^\delta - x^\dagger)\rangle\| \leq 2\alpha\|p\|\|F(x_\alpha^\delta) - F(x^\dagger)\| + \alpha L\|p\|\|x_\alpha^\delta - x^\dagger\|^2.$$

Combining this estimate with (3.13) we deduce

$$\|F(x_\alpha^\delta) - y^\delta)\|^2 + \alpha(1 - L\|p\|)\|x_\alpha^\delta - x^\dagger\|^2 \leq \delta^2 + 2\alpha\|p\|\|F(x_\alpha^\delta) - y\| \leq \delta^2 + 2\alpha\|p\|(\|F(x_\alpha^\delta) - y^\delta\| + \delta),$$

or, rewritten

$$\frac{1}{\alpha}(\|F(x_\alpha^\delta) - y^\delta)\| - \alpha\|p\|)^2 + (1 - L\|p\|)\|x_\alpha^\delta - x^\dagger\|^2 \leq \frac{\delta^2}{\alpha} + \alpha\|p\|^2 + 2\delta\|p\|.$$

If $c_1\delta \leq \alpha \leq c_2\delta$, we obtain (using nonnegativity of the first term on the left-hand side)

$$(1 - L\|p\|)\|x_\alpha^\delta - x^\dagger\|^2 \leq \frac{\delta}{c_1} + c_2\delta\|p\|^2 + 2\delta\|p\|,$$

and hence, (3.12) holds with

$$c = \sqrt{\frac{1 + c_1c_2\|p\|^2 + 2c_1\|p\|}{c_1(1 - L\|p\|)}}.$$

□

We finally mention that a general source condition can be generalized to

$$\exists\, p \in Y: \quad x^\dagger - x^* = (F'(x^\dagger)^*F'(x^\dagger))^\mu p, \tag{3.14}$$

and analogous convergence rate results to the linear case can be shown.

3.2 Construction of Tikhonov-type Regularization Methods

The idea of Tikhonov regularization can easily be generalized with respect to the choice of a regularization functional. With a nonnegative functional $J_R : X \to \mathbb{R}$ one could consider a "Tikhonov-type" regularization via

$$x_\alpha^\delta \in \arg\min_{x \in X} \left[\|F(x) - y^\delta\|^2 + \alpha J_R(x) \right]. \tag{3.15}$$

Such a method is a regularization if the regularization functional J_R has a suitable properties. In particular, if J_R is weakly lower semicontinuous in some topology $\mathcal{T}$, i.e.,

$$J_R(x) \leq \liminf_n J_R(x_n) \qquad \forall\ x_n \to_{\mathcal{T}} x,$$

and if the sub level sets of J_R are precompact in the topology $\mathcal{T}$, the results on existence, stability, and convergence for Tikhonov regularization can be carried over to (3.15) with minor modifications of the proofs, when convergence is considered with respect to the topology $\mathcal{T}$. Since the topology $\mathcal{T}$ need not correspond to the strong or weak topology in a Hilbert space, one can carry out regularization via (3.15) also if X is a metric space. We shall meet this situation for two Banach spaces in the Sections below and for a metric space of shapes in the last chapter.

From this generalization one observes that the main regularizing effect of Tikhonov regularization comes from the fact that the sub level sets of the functional

$$J_\alpha(x) = \|F(x) - y^\delta\|^2 + \alpha J_R(x)$$

are precompact in the topology $\mathcal{T}$, i.e., the regularization acts by compactification. In the case of a Hilbert space, the natural choice for the topology $\mathcal{T}$ is the weak topology, the fact that one finally even obtains strong convergence is a particularity. In a similar setup for Banach spaces one cannot expect strong convergence, as we shall see for total variation regularization below.

3.3 Maximum-Entropy Regularization

Maximum entropy regularization is a method of particular interest for the reconstruction of *probability density functions*, i.e., functions in the space

$$BDF(\Omega) := \{x \in L^1(\Omega) \mid x \geq 0, \int_\Omega x(t)\ dt = 1\}.$$

The (negative) entropy borrowed from physics and information theory is defined as the functional

$$E(x) := \int_\Omega x(t) \log x(t)\ dt, \qquad \forall x \in L^1(\Omega), x \geq 0, \int_\Omega x(t)\ dt = 1. \tag{3.16}$$

For a continuous operator $F : L^1(\Omega) \to Y$ with Y being some Hilbert space, we can consider the regularized problem

$$\|F(x) - y\|^2 + \alpha E(x) \to \min_{x \in PDF(\Omega)}. \tag{3.17}$$

The convergence analysis of maximum entropy regularization (cf. [11, 14]) can be related to the one for Tihonov regularization in Hilbert space with a simple trick: one can find a monotone function $\psi : \mathbb{R}^+ \to \mathbb{R}$ such that

$$E(x) = \int_\Omega x(t) \log x(t)\ dt = \int_\Omega \psi(x(t))^2\ dx.$$

Hence, with the operator

$$\Psi : L^2(\Omega) \to L^1(\Omega), \quad z \mapsto \psi^{-1}(z),$$

can be rewritten as

$$\|F(\Psi(z)) - y\|^2 + \alpha \int_\Omega z(t)^2\ dt \to \min_{z \in L^2(\Omega)}.$$

With suitable assumptions on the solution and the admissible set, one can verify that the new nonlinear operator $F \circ \Phi : L^2(\Omega) \to Y$ satisfies all needed properties for Tikhonov regularization and thus, the convergence (rate) analysis can be carried over, we refer to [14] for further details.

If a prior $x^* \in PDF(\Omega)$ is available, then one often uses the *relative entropy* (or Kullback-Leibler divergence)

$$E^*(x) := \int_\Omega x(t) \log \frac{x(t)}{x^*(t)}\ dt, \qquad \forall x \in L^1(\Omega), x \geq 0, \int_\Omega x(t)\ dt = 1, \tag{3.18}$$

the convergence analysis in this case is similar.

3.4 Total Variation Regularization

Total variation regularization is an approach originally introduced for image restoration (cf. [23]) with the aim of preserving edges in the image, i.e., discontinuities in the solution. Formally the total variation functional can be defined as

$$|u|_{TV} = \int_\Omega |\nabla u|\ dt, \qquad u \in C^1(\Omega).$$

A more rigorous definition is based on the dual form

$$|u|_{TV} := \sup_{\mathbf{g} \in C_0^\infty(\Omega)^d} \int_\Omega u \text{ div } \mathbf{g}\ dt. \tag{3.19}$$

The general definition of the space of functions of bounded variation $BV(\Omega)$ is

$$BV(\Omega) := \{\ u \in L^1(\Omega) \mid |u|_{TV} < \infty\ \}.$$

With this definition, the space $BV(\Omega)$ includes also discontinuous functions. Consider e.g. $\Omega = [-1, 1]$ and, for $R < 1$,

$$u^R(x) = \begin{cases} 1 & \text{if } |x| \leq R \\ 0 & \text{else.} \end{cases}$$

Then,

$$\int_\Omega u \text{ div } g\ dt = \int_{-R}^{R} \frac{dg}{dt}\ dt = g(R) - g(-R).$$

For $\|g\|_\infty \leq 1$, we have $g(R) - g(-R) \leq 2$ and it is easy to construct a function $g \in C_0\infty([-1,1])$ such that $g(R) = 1, g(-R) = -1$ and $\|g\|_\infty \leq 1$. Hence,

$$|u|_{TV} := \sup_{g \in C_0^\infty([-1,1])} [g(R) - g(-R)] = 2.$$

In general, for a function u being equal to 1 in $D \subset\subset \Omega$ and $u = 0$ else, the total variation $|u|_{TV}$ equals the surface area (or curve length) of ∂D.

Total variation regularization is defined via the minimization problem

$$\|F(u) - y\|^2 + \alpha |u|_{TV} \to \min_{u \in BV(\Omega)}.$$

The convergence analysis (cf. [1]) is based on the compact embedding $BV(\Omega) \hookrightarrow L^p(\Omega)$, where $p > 1$ depends on the spatial dimension d. One can use this property to deduce that sub level sets of the regularized functional are compact in the strong topology of $L^p(\Omega)$, and if F is weakly sequentially closed in this topology, one can carry out an analogous convergence proof as for Tikhonov regularization.

In order to obtain further insight, we consider the formal optimality condition in the case $F = Id : BV(\Omega) \to L^2(\Omega)$, i.e., the classical case of denoising considered in [23]. By differentiating formally, we have

$$u - y^\delta = \alpha \text{div} \left(\frac{\nabla u}{|\nabla u|} \right).$$

If u is a continuously differentiable function, the term div $\left(\frac{\nabla u}{|\nabla u|}\right)$ is equal to the mean curvature of the level sets $\{u = \sigma\}$, $\sigma \in \mathbb{R}$. Hence, the optimality condition is a condition on the smoothness of the level sets only, there is no condition on the size of $|\nabla u|$.

Again by formal arguments, we can derive a dual problem for total variation minimization. Consider again the denoising case $F = Id : BV(\Omega) \to L^2(\Omega)$, then the minimization problem to solve is

$$\inf_u \left[\int_\Omega (u - y^\delta)^2 \, dt + \alpha |u|_{TV} \right] = \inf_u \sup_{\mathbf{g}} \left[\int_\Omega (u - y^\delta)^2 \, dt + 2\alpha \int_\Omega u \text{ div } \mathbf{g} \, dt. \right]$$

Under the assumption that we can exchange the inf and sup (in a suitable function space setting), then we obtain

$$\sup_{\mathbf{g}} \inf_u \left[\int_\Omega (u - y^\delta)^2 \, dt + 2\alpha \int_\Omega u \text{ div } \mathbf{g} \, dt. \right]$$

The minimization over u is a strictly convex problem and its unique minimizer can be computed from the first-order optimality conditon as

$$u = y^\delta - \alpha \text{ div } \mathbf{g}.$$

Hence, after eliminating u we end up with the maximization problem

$$\sup_{\mathbf{g}} \left[\alpha^2 \int_\Omega (\text{ div } \mathbf{g})^2 \, dt + 2\alpha \int_\Omega (y^\delta - \alpha \text{ div } \mathbf{g}) \text{ div } \mathbf{g} \, dt \right]$$

Since we can add constant terms without changing the maximizer, the problem is equivalent to

$$-\int_\Omega (\alpha \text{ div } \mathbf{g} - y^\delta)^2 \, dx \to \max_{|\mathbf{g}|_\infty \le \mathbf{1}} .$$

Now let $p := \alpha g$, then we end up with (using the fact that maximization of a functional is equivalent to minimization of the negative functional)

$$\int_\Omega (\text{ div } p - y^\delta)^2 \, dt \to \min_{|p|_\infty \le \alpha} . \tag{3.20}$$

The minimization problem (3.20) is the dual problem of the total variation regularization, if we have computed a solution p, then the primal solution can be computed as $u = y^\delta - \text{ div } p$.

Motivated from the dual problem we can also consider the dual space of BV, namely

$$BV^* := \{ \, q = \text{ div } p \mid p \in L^\infty(\Omega) \, \}$$

with the dual norm

$$\|q\|_{BV^*} := \inf\{\|p\|_\infty \mid q = \text{ div } p\}.$$

Note that (3.20) has the structure of a projection, namely it projects y^δ to the ball of radius α in the dual space BV^*.

The dual problem also allows further insight into the so-called stair-casing phenomenon, i.e., the fact that the total variation regularization favours piecewise constant regularized solutions. Consider for simplicity the one-dimensional case and let $\frac{df}{dx} = y^\delta$. Then, with $q = p - f$, the dual problem can be rewritten as

$$\int_\Omega \left(\frac{dq}{dt}\right)^2 \, dt \to \min \qquad \text{subject to } \; -\alpha \le q + f \le -\alpha. \tag{3.21}$$

Consider formally the associated Lagrangian

$$\mathcal{L}(q; \lambda, \mu) = \int_\Omega \left[\left(\frac{dq}{dt}\right)^2 + \lambda(q + f - \alpha) - \mu(q + f + \alpha) \right] \, dt$$

for positive functions λ and μ. Then the optimality condition becomes

$$-2\frac{d^2 q}{dt^2} + \lambda - \mu = 0$$

and moreover, the constraints

$$\lambda \ge 0, \quad \mu \ge 0, \quad -\alpha \le q + f \le \alpha$$

and the complementarity conditions

$$\lambda(q + f - \alpha) = 0, \quad \mu(q + f + \alpha) = 0.$$

Thus, we have three cases:

1. $q(t) + f(t) = \alpha$, which implies that $\mu(t) = 0$ and $2\frac{d^2 q}{dt^2} = \lambda(t) \ge 0$.

2. $q(t) + f(t) = -\alpha$, which implies that $\lambda(t) = 0$ and $2\frac{d^2q}{dt^2} = -\mu(t) \leq 0$.

3. $q(t) + f(t) \notin \{\alpha, -\alpha\}$, which implies $\lambda(t) = \mu(t) = 0$, and hence, $\frac{d^2q}{dt^2}(t) = 0$.

Note that the third case shows that q is linear in regions where $q + f \notin \{\alpha, -\alpha\}$ and hence, $u = -\frac{dq}{dt}$ is constant.

If y^δ is a piecewise constant function, then f is piecewise linear and thus, the cases 1. and 2. imply that $q = \pm\alpha - f$ is piecewise linear in the respective subregions, and thus, $u = -\frac{dq}{dt}$ is piecewise constant. This means that, together with case 3., u must be a piecewise constant function. Consider for example the special case

$$y^\delta(x) = \begin{cases} 1 & \text{if } |x| \leq R \\ 0 & \text{else.} \end{cases}$$

with $0 < \alpha < R < 1$. By a simple integration we obtain the anti-derivative

$$f(x) = \begin{cases} -R & \text{if } x \leq -R \\ x & \text{if } -R \leq x \leq R \\ R & \text{if } x \geq R \end{cases}$$

Thus, the dual problem becomes

$$\int_\Omega \left(\frac{dq}{dt}\right)^2 \, dt \to \min$$

subject to

$$\begin{array}{ll} -\alpha \leq q - R \leq \alpha & \text{if } x \leq -R \\ -\alpha \leq q + x \leq \alpha & \text{if } -R \leq x \leq R \\ -\alpha \leq q + R \leq \alpha & \text{if } x \geq R \end{array} .$$

Now let

$$\overline{q}(x) = \begin{cases} R - \alpha & \text{if } x \leq -R \\ \frac{\alpha - R}{R} x & \text{if } -R \leq x \leq R \\ \alpha - R & \text{if } x \geq R \end{cases} ,$$

Then $\overline{q}$ satisfies the constraints and

$$\int_\Omega \left(\frac{dq}{dt}\right)^2 \, dt = \frac{2(R-\alpha)^2}{R}.$$

Moreover, for arbitrary q satisfying the constraints we obtain

$$(R - \alpha) - (\alpha - R) \leq q(-R) - q(R) = -\int_{-R}^{R} \frac{dq}{dt} \, dt$$

Hence, from the Cauchy-Schwarz inequality we deduce

$$\int_\Omega \left(\frac{dq}{dt}\right)^2 \, dt \geq \int_{-R}^{R} \left(\frac{dq}{dt}\right)^2 \, dt \geq \frac{1}{2R} \left(\int_{-R}^{R} \left(\frac{dq}{dt}\right) \, dt\right)^2 \geq \frac{2(R-\alpha)^2}{2R}.$$

This shows that $\overline{q}$ is a minimizer of the dual problem and consequently, the regularized solution is given by

$$u(x) = -\frac{d\overline{q}}{dx} = \begin{cases} 0 & \text{if } x \leq -R \\ 1 - \frac{\alpha}{R} & \text{if } -R \leq x \leq R \\ 0 & \text{if } x \geq R \end{cases}$$

Thus, the regularized solution is discontinuous and even has the same discontinuity set as the data, but shrinks the height (in a monotone way with α). It is easy to see by analogous reasoning that for $R < \alpha$, the regularized solution is $u \equiv 0$, i.e., α marks a critical size below which features in the solution will be eliminated. Since such small features are usually due to noise, so the regularization eliminates really parts that one would consider to be noise but maintains important discontinuities. A nice detailed discussion of the properties of solutions in total variation regularization can be found in the book by Meyer [21].

Chapter 4

Parameter Identification

In the following we discuss parameter identification problems in further detail, in particular their numerical solution. In the introductory examples of parameter identification we have observed a particular property of such problems, namely two types of unknowns, the *parameter* a and the *state* u. Parameter and state are linked via an equation, which we formally write as

$$e(u; a) = 0, \qquad e : X \times Q \to Z, . \tag{4.1}$$

for Hilbert space X, Q, and Z. The equation (4.1), which usually represents a system of partial differential equations, is called *state equation*. The solution of the state equation for given a can be interpreted as the direct problem. In typical examples it is reasonable to assume that e is continuously Frechet differentiable and $\frac{\partial e}{\partial u}(u; a) : X \to Z$ is a continuous linear operator with continuous inverse. Hence, by the implicit function theorem we can conclude that (4.1) has a unique solution $u = u(a)$. It is therefore possible to introduce a well-defined operator

$$\Phi : Q \to X, \quad a \mapsto u(a) \text{ solving (4.1)}.$$

Φ is called *parameter-to-solution map*.

The data are related to the state in most examples via a linear *observation operator* $B : X \to Y$, such that $y = Bu$. The observation operator could either be the identity (distributed measurement), a restriction operator to part of the domain (partial distributed measurements), a trace operator to boundary values of the solution (boundary measurements), or a trace operator to final values of a solution in a time-dependent problem. By employing the parameter-to-solution map, we can also define a nonlinear operator $F := B \circ \Phi : Q \to Y$ and formulate the parameter-identification problem in a standard way as the nonlinear operator equation

$$F(a) = y. \tag{4.2}$$

If the operator F is injective, then the parameter a is *identifiable*.

In the case of noisy data, one has several possibilities of a least-squares formulation for the problem. The most frequently used one is the *output least-squares formulation*

$$\|F(a) - y^\delta\|^2 \to \min_{a \in Q}. \tag{4.3}$$

This formulation is equivalent to the constrained problem

$$\|Bu - y^\delta\|^2 \to \min_{(u,a) \in X \times Q} \quad \text{subject to } e(u; a) = 0. \tag{4.4}$$

If we interpret the parameter identification problem as the coupled system

$$Bu = y, \qquad e(u;a) = 0$$

instead, we could also consider the *total least-squares formulation*

$$\|Bu - y^\delta\|^2 + \|e(u;a)\|^2 \to \min_{(u,a)\in X\times Q}. \tag{4.5}$$

The nonlinear operator used in the total least-squares approach is defined on the product space as $\tilde{F} := (B, e) : X \times Q \to Y \times Z$.

4.1 Derivatives and the Adjoint Method

For typical numerical solution methods one always needs to compute derivatives of the nonlinear operator F or $\tilde{F}$ and the associated least-squares functionals, respectively.

Using the chain rule and the linearity of the observation operator we obtain that

$$F'(a) = B \circ \Phi'(a),$$

and since $e(\Phi(a), a) = 0$ we have

$$\frac{\partial e}{\partial u}(\Phi(a), a)\Phi'(a) + \frac{\partial e}{\partial a}(\Phi(a), a) = 0,$$

i.e., since we have assumed that $\frac{\partial e}{\partial u}$ is regular,

$$\Phi'(a) = -\frac{\partial e}{\partial u}(\Phi(a), a)^{-1}\frac{\partial e}{\partial a}(\Phi(a); a).$$

Altogether, the derivative of the operator F is given by

$$F'(a) = -B \circ \frac{\partial e}{\partial u}(\Phi(a); a)^{-1} \circ \frac{\partial e}{\partial a}(\Phi(a); a).$$

Hence, in order to evaluate the directional derivative $F'(a)h$, we have to solve the linearized problem

$$\frac{\partial e}{\partial u}(\Phi(a); a)[\Phi'(a)h] + \frac{\partial e}{\partial a}(\Phi(a); a)h = 0 \tag{4.6}$$

and then apply the observation operator to the solution. Note that the linearized problem (4.6) is a system of (linear) differential equations. Consider for example $X = H_0^1(\Omega)$, $Z = H^{-1}(\Omega)$ and

$$e(u;a) := -\text{ div } (a\nabla u) - f, \qquad B = Id : H_0^1(\Omega) \to L^2(\Omega), \tag{4.7}$$

then the derivatives are given by

$$\frac{\partial e}{\partial u}(u;a)v = -\text{div } (a\nabla v), \qquad \frac{\partial e}{\partial a}(u;a)h = -\text{div } (h\nabla u).$$

Hence, the linearized problem is the solution of the linear partial differential equation

$$-\text{div } (a\nabla v) = \text{div } (h\nabla u),$$

and its solution is equal to $\Phi'(a)h = v$. Thus, in order to compute a directional derivative, one has to solve a linear partial differential equation. In order to compute the full Frechet derivative $F'(a)$ one has to solve an equation for each h.

With the formula for $F'(a)$ it is easy to compute the derivative of the output least-squares functional

$$J_O(a) := \|F(a) - y^\delta\|^2$$

as

$$\begin{aligned} J_O'(a)h &= 2\langle F(a) - y^\delta, F'(a)h\rangle = 2\langle F'(a)^*(F(a) - y^\delta), h\rangle \\ &= -2\langle \frac{\partial e}{\partial a}(\Phi(a);a)^*(\frac{\partial e}{\partial u}(\Phi(a);a)^*)^{-1}B^*(F(a) - y^\delta), h\rangle. \end{aligned}$$

Hence,

$$J_O'(a)h = -2\frac{\partial e}{\partial a}(\Phi(a);a)^*(\frac{\partial e}{\partial u}(\Phi(a);a)^*)^{-1}(F(a) - y^\delta).$$

Using this formula involving the adjoints of the derivatives of e, we can directly compute the gradient of the functional J_O as $J_O'(a) = -2\frac{\partial e}{\partial a}(\Phi(a);a)^*w$, where w is the solution of the *adjoint equation*

$$\frac{\partial e}{\partial u}(\Phi(a);a)^*w = F(a) - y^\delta.$$

For example (4.7) with $X = H_0^1(\Omega)$ we can compute the adjoint via

$$\begin{aligned} \langle \frac{\partial e}{\partial u}(u;a)v, w\rangle &= -\int_\Omega \text{div } (a\nabla v)w \; dx \\ &= \int_\Omega a\nabla v \cdot \nabla w \; dx = -\int_\Omega \text{div } (a\nabla w)v \; dx \\ &= \langle v, \frac{\partial e}{\partial u}(u;a)^*w\rangle. \end{aligned}$$

Thus, the adjoint equation is the linear partial differential equation

$$-\text{ div } (a\nabla w) = u - y^\delta. \tag{4.8}$$

For complicated parameter identification problems, the direct computation of the adjoint is rather involved. An attractive alternative is a computation via the derivatives of the Lagrangian

$$\mathcal{L}(u,a,w) := \|Bu - y^\delta\|^2 + \langle e(u;a), w\rangle. \tag{4.9}$$

It is easy to see that

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial u}(u,a,w) &= 2B^*(Bu - y^\delta) + \frac{\partial e}{\partial u}(u;a)^*w \\ \frac{\partial \mathcal{L}}{\partial a}(u,a,w) &= \frac{\partial e}{\partial a}(u;a)^*w \\ \frac{\partial \mathcal{L}}{\partial w}(u,a,w) &= e(u;a). \end{aligned}$$

Thus, for given $a \in Q$, the solution $u \in X$ of $\frac{\partial \mathcal{L}}{\partial w}(u,a,w) = 0$ equals $\Phi(a)$. Let, for given u and a, w be the solution of $\frac{\partial \mathcal{L}}{\partial u}(u,a,w) = 0$, then

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial a}(u,a,w) &= \frac{\partial e}{\partial a}(\Phi(a);a)^* w \\ &= -2\frac{\partial e}{\partial a}(\Phi(a);a)^*(\frac{\partial e}{\partial u}(\Phi(a);a)^*)^{-1}B^*(B\Phi(a) - y^\delta) \\ &= F'(a)^*(F(a) - y^\delta).\end{aligned}$$

Hence, we can compute the derivative of the least-squares functional directly from the Lagrangian by subsequently solving the equations $\frac{\partial \mathcal{L}}{\partial w} = 0$, $\frac{\partial \mathcal{L}}{\partial u} = 0$ and evaluating $\frac{\partial \mathcal{L}}{\partial a}$.

In an analogous way we can compute derivatives of the operator $\tilde{F}$ as

$$\begin{aligned}\frac{\partial \tilde{F}}{\partial u}(u,a) &= (B, \frac{\partial e}{\partial u}(u;a)), \\ \frac{\partial \tilde{F}}{\partial a}(u,a) &= (0, \frac{\partial e}{\partial a}(u;a)).\end{aligned}$$

The derivative of the total least-squares functional

$$J_T(u;a) = \|\tilde{F}(u;a) - (y^\delta, 0)\|^2 = \|Bu - y^\delta\|^2 + \|e(u;a)\|^2$$

is given by

$$J_T'(u;a)(v,h) = 2\langle Bv, Bu - y^\delta\rangle + 2\langle \frac{\partial e}{\partial u}(u;a)v; e(u;a)\rangle + 2\langle \frac{\partial e}{\partial a}(u;a)v; e(u;a)\rangle.$$

The terms involved in the computation of the derivative J_T' are again the same as appearing in the derivative of J_O'.

4.2 Regularization

Under usual assumptions, one has to expect that a parameter identification problem is ill-posed (and most parameter identification problems are actually ill-posed). Therefore it is a natural first step to investigate the regularization of parameter identification problems. For this sake one needs to understand on which variable the regularization should act. From the viewpoint of (4.2) and (4.3) it seems clear that any regularization method for nonlinear ill-posed problems can be applied directly, with regularization acting on the only variable $a \in Q$. For the formulation (4.5) it is not obvious whether one should also incorporate regularization on u. However, it can be shown that such an additional regularization is not necessary due to the inherent well-posedness of the problem (respectively equation (4.1)) with respect to the state u.

Tikhonov Regularization

We start with the investigation of Tikhonov regularization. From (4.3), we arrive at the regularized problem

$$\|F(a) - y^\delta\|^2 + \alpha\|a - a^*\|^2 \to \min_{a \in Q}, \tag{4.10}$$

or, equivalently,

$$\|Bu - y^\delta\|^2 + \alpha\|a - a^*\|^2 \to \min_{(u,a)\in X\times Q} \quad \text{subject to } e(u;a) = 0. \tag{4.11}$$

The condition of weak sequential closedness of the operator F needed for the analysis of Tikhonov regularization is equivalent to the weak sequential closedness of the parameter-to-solution map Φ, because the continuous linear observation operator will preserve this property.

The Tikhonov regularization of the total least-squares formulation (4.5) is

$$\|Bu - y^\delta\|^2 + \|e(u;a)\|^2 + \alpha\|a - a^*\|^2 \to \min_{(u,a)\in X\times Q}. \tag{4.12}$$

The condition of weak sequential closedness of the operator $\tilde{F} := (B, e) : X \times Q \to Y \times Z$ is equivalent to weak sequential closedness of the equation operator e. A possible advantage of the output least-squares formulation is a natural way of dealing with perturbations in the equation. If, instead of $e(u, a)$, a perturbation $e(u, a) + f^\delta$ with $\|f^\delta\| \le \delta$ is given, we can analyze convergence in the same way as for standard regularization.

In order to gain some insight into the structure of the regularized problem, we consider the example (4.7). For simplicity we consider $a-a^* \in H_0^1(\Omega)$ (which is indeed a regularization for $d = 1$) with the norm

$$\|b\|_{H_0^1} := \sqrt{\int_\Omega |\nabla b|^2 \, dt}.$$

The output least-squares formulation is equivalent to

$$\begin{aligned} \int_\Omega (u - y^\delta)^2 \, dt + \alpha \int_\Omega |\nabla a - \nabla a^*|^2 \, dt \to & \min_{(u,a)\in H_0^1(\Omega)\times H_0^1(\Omega)} \\ \text{subject to} \qquad -\ \text{div}\,(a\nabla u) = f \qquad & \text{in } \Omega. \end{aligned}$$

Every global minimizer of the Tikhonov functional is also a saddle-point of the Lagrangian

$$\mathcal{L}_\alpha(u, a, w) = \int_\Omega (u - y^\delta)^2 \, dt + \alpha \int_\Omega |\nabla a - \nabla a^*|^2 \, dt + \int_\Omega (a\nabla u \cdot \nabla w - fw) \, dt, \tag{4.13}$$

where we have used Gauss' Theorem to convert the state equation to its weak form. Thus, the optimality condition becomes

$$\begin{aligned} 0 = \frac{\partial \mathcal{L}_\alpha}{\partial a}(u, a, w) &= -2\alpha \ \text{div}\,(\nabla(a - a^*)) + \nabla u \cdot \nabla w, \\ 0 = \frac{\partial \mathcal{L}_\alpha}{\partial u}(u, a, w) &= -\ \text{div}\,(a\nabla w) + 2(u - y^\delta), \\ 0 = \frac{\partial \mathcal{L}_\alpha}{\partial w}(u, a, w) &= -\ \text{div}\,(a\nabla u) - f. \end{aligned}$$

Thus, the regularized solution can (at least in principle) be computed as the solution of a system of partial differential equations.

Total Variation Regularization

In several applications, the unknown parameter can be modeled as a piecewise constant function, but with unkown function values and unknown discontinuity sets. An example is the reconstruction of material parameters on domains that consist of a mixture of different materials (and each material is characterized by a specific scalar value). Under these conditions it is natural to use total variation regularization for the parameter identification problem, i.e., to minimize,

$$\|F(a) - y^\delta\|^2 + \alpha |a|_{TV} \to \min_{a \in Q}, \tag{4.14}$$

As we have seen above, the total variation functional favours piecewise constant solutions and the discontinuity set of the exact parameter is approximated well by the regularized solution.

Iterative Regularization by the Landweber Method

The simplest iterative regularization method, namely Landweber iteration, is given in the abstract setting as

$$a^{k+1} = a^k - \tau^k F'(a^k)^*(F(a^k) - y^\delta).$$

In terms of the funcional J_O and the associated Lagrangian we can rewrite the iteration as

$$a^{k+1} = a^k - \frac{\tau^k}{2} J_O'(a^k) = a^k - \frac{\tau^k}{2} \frac{\partial \mathcal{L}}{\partial a}(u^k, a^k, w^k),$$

for a suitable damping parameter $\tau^k > 0$, where $u^k = \Phi(a^k)$ is determined as the solution of

$$\frac{\partial \mathcal{L}}{\partial w}(u^k, a^k, w^k) = e(u^k; a^k)$$

and subsequently w^k as the solution of

$$\frac{\partial \mathcal{L}}{\partial u}(u^k, a^k, w^k) = 2B^*(Bu^k - y^\delta) + \frac{\partial e}{\partial u}(u^k; a^k)^* w^k = 0.$$

Hence, the computation of one iteration step of the Landweber iteration consists of three parts: First of all, given a^k the state equation is solved to compute u^k, then the adjoint equation is solved to compute w^k and finally, $\frac{\partial \mathcal{L}}{\partial a}(u^k, a^k, w^k) = \frac{\partial e}{\partial a}(u^k, a^k)^* w^k$ is evaluated to determine the update in the iteration procedure.

We again take a closer look at the iteration procedure for (4.7). The Lagrangian is given by

$$\mathcal{L}(u, a, w) = \int_\Omega (u - y^\delta)^2 \, dt + \int_\Omega a \nabla u \cdot \nabla w \, dt, \tag{4.15}$$

and hence, in order to compute the update we have to solve the partial differential equations

$$\begin{aligned} 0 = \frac{\partial \mathcal{L}_\alpha}{\partial w}(u^k, a^k, w^k) &= -\operatorname{div}(a^k \nabla u^k) - f \\ 0 = \frac{\partial \mathcal{L}_\alpha}{\partial u}(u^k, a^k, w^k) &= -\operatorname{div}(a^k \nabla w^k) + 2(u^k - y^\delta). \end{aligned}$$

The update formula has to be carried out in the Hilbert space $H_0^1(\Omega)$, i.e., in weak form we have

$$\langle a^{k+1} - a^k, \varphi \rangle = -\frac{\tau^k}{2} J_O'(a^k)\varphi, \qquad \forall\ \varphi \in H_0^1(\Omega).$$

If we choose the same scalar product as above, then

$$\langle a^{k+1} - a^k, \varphi \rangle = \int_\Omega \nabla(a^{k+1} - a^k) \cdot \nabla \varphi \, dt = - \int_\Omega \varphi \, \text{div} \, \nabla(a^{k+1} - a^k) \, dt.$$

Hence, the update involves the solution of another partial differential equation of the form

$$- \text{div} \, \nabla(a^{k+1} - a^k) = -\frac{\tau^k}{2} \nabla u^k \cdot \nabla w^k.$$

Note that once the gradient is known, it is also easy to use a quasi-Newton approach such as BFGS with little extra effort.

Iterative Regularization by the Levenberg-Marquardt Method

The last regularization approach we discuss is the Levenberg-Marquardt method, where the iterates are computed from

$$(F'(a^k)^* F'(a^k) + \alpha^k I)(a^{k+1} - a^k) = -F'(a^k)^*(F(a^k) - y^\delta),$$

which is equivalent to the minimization problem

$$J^k(a) := \|F(a^k) - y^\delta + F'(a^k)(a - a^k)\|^2 + \alpha^k \|a - a^k\|^2 \to \min_{a \in Q}.$$

This minimization is equivalent to

$$\begin{aligned} &\|Bu^k - y^\delta + Bv\|^2 + \alpha^k \|a - a^k\|^2 \to \min_{(v,a) \in X \times Q} \\ &\text{subject to } \frac{\partial e}{\partial u}(u^k; a^k)v + \frac{\partial e}{\partial a}(u^k; a^k)(a - a^k) = 0, \end{aligned}$$

where $u^k = \Phi(a^k)$ The optimality condition for this constrained problem are given by the system

$$\begin{aligned} 0 &= 2\alpha^k(a^{k+1} - a^k) + \frac{\partial e}{\partial a}(u^k; a^k)^* w^k \\ 0 &= 2B^*(Bu^k - y^\delta + Bv^k) + \frac{\partial e}{\partial a}(u^k; a^k)^* w^k \\ 0 &= \frac{\partial e}{\partial u}(u^k; a^k)v^k + \frac{\partial e}{\partial a}(u^k; a^k)(a^{k+1} - a^k) \end{aligned}$$

to be solved for $a^{k+1} \in Q$, $v^k \in X$, $w^k \in Z$. Hence, the realization of the Levenberg-Marquardt method enforces the solution of a linear system of differential equations, which is close to the linearization of the optimality conditions for Tikhonov regularization.

4.3 Large Scale Problems

We finally discuss the solution of large scale problems such as the examples of electrical impedance tomography and inverse scattering discussed before. In theory, one assumes to measure the full Dirichlet-to-Neumann map or the full far-field pattern, but in practice one clearly can measure only a finite number of evaluations of the maps. E.g., in impedance

tomography, it is reasonable to measure $\Lambda_a(f_j)$ for $j = 1, \ldots, N$, and N being a very large number. This means we have to solve N state equations

$$-\operatorname{div}(a\nabla u^j) = 0$$

with boundary values $u_j = f_j$.

The general form corresponding to such a case is a state $u = (u^1, \ldots, u^N)$ with state equation

$$e(u; a) = (e_1(u^1; a), \ldots, e_N(u^N; a)) = 0 \tag{4.16}$$

and observation operator

$$Bu = (B_1 u^1, \ldots, B_N u^N). \tag{4.17}$$

The derivative of the associated output least-squares functional in this case can be computed again by the adjoint method, but since u^j only appears in the j-th equation we obtain a very peculiar structure. It is easy to see that

$$F'(a)^*(F(a) - y^\delta) = \sum_{j=1}^{N} \frac{\partial e_j}{\partial a}(u^j; a)^* w^j,$$

where the adjoint state is the solution of

$$\frac{\partial e_j}{\partial u}(u^j; a)^* w^j + B_j^*(B_j u^j - y_j^\delta) = 0.$$

and the state is just determined from $e_j(u^j; a) = 0$.

The special structure of the derivative can be used to compute gradients with reasonable memory consumption. Note that if N is large and the discretization is fine, the unknowns for the state variables u^j and the adjoint states w^j may produce a very high number of unknowns. Therefore, it seems advantageous not to compute and store all of them at the same time, but to compute them in a sequential way (or separately distributed on several processors). Such a computation is easy from the above form of the gradient, we start with $g_0 := 0$ and then use the recursion

$$g_j := g_{j-1} + \frac{\partial e_j}{\partial a}(u^j; a)^* w^j, \qquad j = 1, \ldots, N,$$

with states and adjoint states u^j and w^j as above. In this way we only need the memory for u^1 and w^1, which can later be used for u^j and w^j subsequently.

With this way of computing the gradient it is straight-forward to realize the Landweber iteration, with the setting $a^{k,0} = a^k$ we compute

$$a^{k,j} = a^{k,j-1} + \tau^j \frac{\partial e_j}{\partial a}(u^{k,j}; a^k)^* w^{k,j}, \qquad j = 1, \ldots, N$$

to obtain the new iterate $a^{k+1} = a^{k,N}$. Here $u^{k,j}$ and $w^{k,j}$ are the solutions of

$$e(u^{k,j}; a^k) = 0, \qquad \frac{\partial e_j}{\partial u}(u^{k,j}; a^k)^* w^{k,j} + B_j^*(B_j u^{k,j} - y_j^\delta) = 0.$$

Instead of the additive splitting in the computation of the update a^{k+1} one could also use a multiplicative splitting, i.e.,

$$a^{k,j} = a^{k,j-1} + \tau^j \frac{\partial e_j}{\partial a}(u^j; a^{k,j-1})^* w^j, \qquad j = 1, \ldots, N$$

now with $u^{k,j}$ and $w^{k,j}$ being the solutions of

$$e(u^{k,j}; a^{k,j-1}) = 0, \qquad \frac{\partial e_j}{\partial u}(u^{k,j}; a^{k,j-1})^* w^{k,j} + B_j^*(B_j u^{k,j} - y_j^\delta) = 0.$$

This approach is called *Landweber-Kaczmarz method* (cf. [19]), for some practical problems one observes even better convergence properties for this method than for the simple Landweber iteration. We mention that the relation between Landweber and Landweber-Kaczmarz is of the same type as between Jacobi and Gauss-Seidel iteration for linear systems.

The Kaczmarz-type approach also offers the possibility to perform Newton-type methods with reasonable memory consumption, for example one can perform a Levenberg-Marquardt type approach by freezing $u^{k,m}$ for $m \neq j$ and coupling the iterations in a cyclic way (cf. [6]).

Chapter 5

Shape Reconstruction Problems

In this section we shall deal with the solution of parameter identification problems, where the unknown variable is a shape or geometry in $\mathbb{R}^d$. Shapes can be considered as sets with regular boundary and therefore we may perform standard set operations like unions or intersections. However, there is no way to make a class of shapes into a linear space in general, but only with severe restrictions. An obvious way of solving a problem in a linear space instead of a problem on a class of shapes is to use parametrization (e.g. as piecewise graphs, by polar coordinates, or locally around a given shape). Since the parametrization is usually represented by a function on a fixed set, one can just minimize over all such functions in an appropriate Hilbert or Banach space. This allows to use standard methods as discussed above, but strongly limits the class of admissible shapes.

5.1 Shape Sensitivity Analysis

The main idea of shape sensitivity analysis is to consider "natural deformations" of shapes and inspect the corresponding variations of the objective functional. The general setup in the following is the minimization of

$$J(\Omega) \to \min_{\Omega \in \mathcal{K}},$$

where $\mathcal{K}$ is a suitable class of compact subsets of $\mathbb{R}^d$, with regular boundary.

There are two different ways of deriving shape sensitivities (both leading to the same result), namely via "direct deformations" or via the "speed method". We shall follow the latter, since this approach fits very well to the level set method, which we will discuss below as a possible solution method for shape optimization problems. For a detailed discussion of shape derivatives we refer to [10].

Before considering shapes we illustrate the idea of the speed method when applied to Gateaux-derivatives in linear spaces. In order to compute the directional derivative of a functional $J : \mathcal{U} \to \mathbb{R}$, we have so far considered the variation between the values of J at $\overline{u} \in \mathcal{U}$ and at its local deformation $\overline{u} + tv$. Alternatively, we could define $u(t) = \overline{u} + tv$ by

$$\frac{du}{dt} = v, \quad u(0) = \overline{u},$$

which is an initial value problem for an ordinary differential equation in $\mathcal{U}$. Using the chain

rule, we can then compute

$$\frac{d}{dt}J(u(t)) = J'(u(t))\frac{du}{dt} = J'(u(t))v.$$

In particular,

$$\frac{d}{dt}J(u(t))\Big|_{t=0} = J'(\overline{u})v,$$

i.e., we obtain the directional derivative at $\overline{u}$ by evaluating the time derivative of $J(u(t))$ at time $t = 0$.

In a similar way, we can define derivatives of shapes. Let $V : \mathbb{R}^d \to \mathbb{R}^d$ be a given velocity field and define $x(t)$ via

$$\frac{dx}{dt}(t) = V(x(t)), \quad x(0) = \overline{x}, \tag{5.1}$$

for each $\overline{x} \in \mathbb{R}^d$. We can then define the shape sensitivity

$$dJ(\overline{\Omega}; V) := \left(\frac{d}{dt}J(\Omega(t))\right)\Big|_{t=0},$$

where

$$\Omega(t) = \{x(t) \mid x(0) \in \overline{\Omega}\}.$$

Note that the main difference to derivatives in linear spaces is that the deformation defined by the ODE (5.1) is nonlinear, since V depends on x itself.

We start with some examples. Let $g : \mathbb{R}^d \to \mathbb{R}$ be a continuously differentiable function and define

$$J(\Omega) := \int_\Omega g(x)\ dx.$$

Then, by change of variables

$$\begin{aligned} J(\Omega(t)) &= \int_{\Omega(t)} g(x)\ dx \\ &= \int_\Omega g(x_y(t))|M_y|\ dy \end{aligned}$$

where $x_y(t)$ is defined by

$$\frac{dx_y}{dt}(t) = V(x_y, t), \quad x_y(0) = y \in \Omega$$

and $M_y = \det \frac{\partial x_y}{\partial y}$. Hence, the time derivative can be computed as

$$\frac{d}{dt}J(\Omega(t)) = \int_\Omega \overline{v}\nabla g(x_y)\frac{\partial x_y}{\partial t}|M_y|\ dy + \int_\Omega g(x_y)\frac{\frac{\partial M_y}{\partial t}M_y}{|M_y|}dy.$$

For the derivative of the determinant we have

$$\begin{aligned}\frac{\partial M_y}{\partial t} &= \frac{\partial}{\partial t}\left(\sum_{(i_1,\dots i_d)\in\Pi(d)}(-1)^{i_1+\dots+i_d}\prod_{k=1}^{d}\frac{\partial (x_y)_k}{\partial y_{i_k}}\right)\\ &= \left(\sum_{(i_k)\in\Pi(d)}(-1)^{\sum i_k}\sum_j\frac{\partial^2 (x_y)_j}{\partial y_{i_j}\partial t}\prod_{l\neq j}^{d}\frac{\partial (x_y)_l}{\partial y_{i_l}}\right)\\ &= \sum_{(i_k)\in\Pi(d)}(-1)^{\sum i_k}\sum_j\frac{\partial V_j}{\partial y_{i_j}}\prod_{l\neq j}^{d}\frac{\partial (x_y)_l}{\partial y_{i_l}}\end{aligned}$$

For $t=0$, we have $\frac{\partial x_y}{\partial y}=I, M_y=1$, and this implies

$$\frac{\partial M_y}{\partial t}=\sum_j\frac{\partial V_j}{\partial y_j}=\text{ div }(V)$$

As a consequence, we have

$$\begin{aligned}\frac{d}{dt}J(\Omega(t))\Big|_{t=0} &= \int_\Omega\left(\nabla g(x_y)\frac{\partial x_y}{\partial t}\right)\Big|_{t=0}dy+\int_\Omega\Big(g(x_y)\text{ div }V(x_y)\Big)\Big|_{t=0}dy\\ &= \int_\Omega\Big(\nabla g(y)V(y)+g(y)\text{ div }V(y)\Big)dy\\ &= \int_\Omega\text{ div }\Big(g(y)V(y)\Big)dy\\ &= \int_{\partial\Omega}g(y)V(y).n\ ds,\end{aligned}$$

where n denotes the unit outer normal on $\partial\Omega$. I.e., the shape sensitivity is a linear functional fo V concentrated on $\partial\Omega$. Another key oberservation is that the shape sensitivity $J'(\Omega)V:=\frac{d}{dt}J(\Omega(t))|_{t=0}$ depends on $V.n|_{\partial\Omega}$ only, while it is completely independent of the values for V inside Ω and of its tangential component. Consequently, we may directly consider variations of $\partial\Omega$ with a velocity $V=V_n.n$, where V_n is a scalar speed function. The shape sensitivity then becomes

$$J'(\Omega)V_n=\int_{\partial\Omega}g.V_n\ ds.$$

The statement that the shape sensitivity is a linear functional of $V.n$ only holds for very general classes of objective functionals, it is usually known as the "Hadamard-Zolésio Structure Theorem". The independence of the shape sensitivity on tangential components is clear from geometric intuition, since those components correspond to a change of parametrization only. The independence on values of V in the interior of Ω seems obvious, too, since they do not change the domain of integration in the objective functional.

In most typical applications of shape optimization, the objective functional depends on a state variable u that satisfies a partial differential equation related to Ω. This relation can arise in several ways, e.g.

1. u solves a partial differential equation in a domain $\Omega\subset\subset D$, and $\partial\Omega$ is the discontinuity set for some of the parameters. A simple example is the optimal design of two conductive

materials, where the conductivity a takes two different values, i.e.,

$$a(x) = \begin{cases} a_1 & x \in \Omega \\ a_2 & x \in D \backslash \Omega. \end{cases}$$

A typical shape optimization problem consists in the optimization of some functional $J(\Omega) = \tilde{J}(u_\Omega)$, where u_Ω solves

$$-\text{ div } (a \nabla u_\Omega) = 0.$$

2. u solves a partial differential equation in Ω and satisfies a boundary condition on $\partial\Omega$.

3. u solves a partial differential equation on the surface of $\partial\Omega$.

The general structure fo such problems is

$$J(\Omega) = \tilde{J}(u_\Omega, \Omega) \to \min_\Omega$$

subject to

$$e(u_\Omega, \Omega) = 0,$$

where e denotes the partial differential equation. In this case we have to use the chain rule and an implicit function theorem to compute the shape sensitivity. Let $\Omega(t)$ be as above and let $u(t)$ denote the solution of

$$e(u(t), \Omega(t)) = 0$$

with $\Omega(t)$ given. Then the shape sensitivity of J is given by

$$\begin{aligned} J'(\Omega)V &= \frac{d}{dt} J(\Omega(t))\Big|_{t=0} \\ &= \frac{d}{dt}\Big(\tilde{J}(u(t), \Omega(t))\Big)\Big|_{t=0} \\ &= \frac{\partial \tilde{J}}{\partial u}(u(0), \Omega(0))u'(0) + \frac{\partial \tilde{J}}{\partial \Omega}(u(0), \Omega(0))V. \end{aligned}$$

Here $\frac{\partial \tilde{J}}{\partial u}$ denotes the (Gateaux-)derivative of $\tilde{J}$ with respect to u (for Ω fixed) and $\frac{\partial \tilde{J}}{\partial \Omega}$ denotes the shape sensitivity of $\tilde{J}$ with respect to Ω (for u fixed). Due to the chain rule we obtain for $u'(0) = \frac{d}{dt} u(t)|_{t=0}$ the equation

$$0 = \frac{d}{dt} e(u(t), \Omega(t)) = \frac{\partial e}{\partial u}(u(t), \Omega(t))u'(t) + \frac{\partial e}{\partial \Omega}(u(t), \Omega(t))V.$$

Here, $\frac{\partial e}{\partial \Omega}(u, \Omega(t))V = \frac{d}{dt} e(u, \Omega(t))$, for u fixed, i.e., it means a generalization of shape sensitivities from functionals to operators. The function $u' = u'(0)$ is usually called "shape derivative".

We shall discuss the computation of shape derivatives for two examples. First, consider the maximization of current for a conductive material. The objective is given by

$$J(\Omega) = -\int_\Gamma a \frac{\partial u_\Omega}{\partial n}\, ds,$$

where $\Gamma \subset D, \Omega \subset\subset D$ and u solves

$$-\text{ div } (a\nabla u) = f, \quad \text{in } D$$

with homogeneous boundary values $u = 0$ on ∂D. Here, f is a given function and a is defined as above, i.e.

$$a(x) = \begin{cases} a_1 & x \in \Omega \\ a_2 & x \in D\backslash\Omega. \end{cases}$$

The shape sensitivity is then given by (note that $\Omega \subset\subset D$ and thus $a = a_2$ on ∂D)

$$J'(\Omega)V = -\int_\Gamma a_2 \frac{\partial u'}{\partial n} ds,$$

where u' is the shape derivative corresponding to the above state equation. In order to compute the shape derivative u', we consider the state equation in its weak form, i.e. we seek $u \in H_0^1(D)$ satisfying

$$\int_D a\nabla u\nabla v \; dx = \int_D fv \; dx \quad \forall v \in H_0^1(D)$$

We can write the left-hand side as

$$< v, e(u,\Omega) >= \int_D a_2\nabla u\nabla v \; dx + \int_\Omega (a_1 - a_2)\nabla u\nabla v \; dx.$$

The derivative with respect to u is given by

$$\frac{\partial e}{\partial u}(u,\Omega)u' = \int_D a_2\nabla u'\nabla v \; dx + \int_\Omega (a_1 - a_2)\nabla u'\nabla v \; dx = \int_D a\nabla u'\nabla v \; dx.$$

In order to compute the derivative with respect to Ω, we can use the above results on shape sensitivities for the functional $\int_\Omega g \; dx$, now with $g = (a_1 - a_2)\nabla u.\nabla v$. Thus,

$$\frac{\partial e}{\partial \Omega}(u,\Omega)V = \int_{\partial\Omega} \Big((a_1 - a_2)\nabla u.\nabla v\Big) V.n \; ds \quad \forall v \in H_0^1(D).$$

As for standard optimal design problems, we can also employ the adjoint method to compute the shape sensitivity. For this sake, let $u^* \in H_0^1(D)$ be the unique weak solution of

$$\int_\Gamma a_2 \frac{\partial w}{\partial n} dx = \int_D a\nabla w\nabla u^* \; dx \quad \forall w \in H_0^1(D).$$

Then we obtain

$$-\int_\Gamma a_2 \frac{\partial u'}{\partial n} ds = -\int_D a\nabla u'\nabla u^* \; dx = \int_{\partial\Omega} \Big((a_1 - a_2)\nabla u.\nabla u^*\Big) V.n \; ds,$$

i.e., the shape sensitivity is again a functional of $V.n$ concentrated on $\partial\Omega$.

Our second example is the shape derivative for a state equation with Dirichlet boundary condition, i.e.

$$\begin{aligned} \Delta u &= f \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$

It is easy to show that

$$\Delta u' = 0 \quad \text{in } \Omega.$$

For the boundary condition, let $y \in \partial\Omega$ and let $\frac{dx}{dt}(t) = V(x(t)), x(0) = y$. Then $u(x(t)) = 0$ for all t and thus

$$\frac{d}{dt}u(x(t)) = u'(x(t)) + \nabla u(x(t)).V(x(t)) = 0.$$

Hence, u' satisfies

$$u' = -\nabla u.V \quad \text{on } \partial\Omega.$$

We finally notice that second derivatives, so-called shape Hessians can be computed by applying the same technique as for shape sensitivities to $J'(\Omega)V$, now with a second velocity W.

5.2 Level Set Methods

Level set methods recently received growing attention in shape optimization due to their capabilities of solving shape optimization problems without parametrizations. The main idea of the level set method is to represent a shape as

$$\Omega(t) = \{\phi(.,t) < 0\},$$

where $\phi : \mathbb{R}^d \times \mathbb{R}^+ \to \mathbb{R}$ is a suitable continuous function, ideally the signed distance function to $\partial\Omega$ (i.e., equal to the distance between x and $\partial\Omega$ if $x \in \mathbb{R}^d \backslash \Omega$, and equal to the negative distance if $x \in \Omega$). For an appropriate ϕ we have that

$$\partial\Omega(t) = \{\phi(.,t) = 0\}.$$

Now consider the motion of points in $\Omega(t)$ by $\frac{dx}{dt} = V(x)$. Then we obtain from the chain rule for $x(t) \in \partial\Omega(t)$

$$0 = \frac{d}{dt}\phi(x(t),t) = \frac{\partial\phi}{\partial t} + V.\nabla\phi = 0,$$

i.e., ϕ can be determined by solving a transport equation. As we have seen above, the most interesting case is the one of a motion in normal direction on $\partial\Omega(t)$, i.e., $V = V_n.n$. In order to use such a velocity in the level set method, we have to express the normal in terms of the level set function ϕ. Assume that $\{\tilde{x}(s,t) | s \in (-\epsilon, \epsilon)\}$ is an arc on $\partial\Omega(t)$, locally parametrized by s around $x(t) = \tilde{x}(0,t)$. Then

$$0 = \frac{d}{ds}\phi(\tilde{x}(s,t),t) = \nabla\phi(\tilde{x}(s,t),t)\frac{\partial\tilde{x}}{\partial s}.$$

Since $\frac{\partial\tilde{x}}{\partial s}$ can be any tangential direction, we obtain that $\nabla\phi$ is a normal direction, and one obtains the unit normal as

$$n(s,t) = \frac{\nabla\phi}{|\nabla\phi|}(\tilde{x}(s,t),t).$$

Using these formulas together with the transport equation for ϕ, we obtain the Hamilton-Jacobi equation

$$\frac{\partial\phi}{\partial t} + V_n|\nabla\phi| = 0 \tag{5.2}$$

for ϕ. One can show that the motion of $\Omega(t)$ is determined by

$$\Omega(t) = \{\phi(.,t) < 0\}$$

if ϕ is a solution of (5.2) in $\mathbb{R}^d \times \mathbb{R}^+$ where V_n is an arbitrary extension from $\{\phi(.,0) < 0\}$ to $\mathbb{R}^d$.

For further details and applications of the level set method we refer to the monograph by Osher and Fedkiw [22], and for the application of level set methods to shape optimization and reconstruction as well as further links to literature we refer to the survey paper [7].

5.2.1 Computing Shape Sensitivities by Level Set Methods

Using the level set method, we can formally compute shape sensitivities in a simple way. Consider again the functional

$$J(\Omega) = \int_\Omega g(x)\ dx$$

and let $\partial\Omega(t)$ move with normal speed V_n. Then we obtain

$$\begin{aligned} J(\Omega(t)) &= \int_{\{\phi(.,t)<0\}} g(x)\ dx \\ &= \int_{\mathbb{R}^d} H(-\phi(x,t))g(x)\ dx, \end{aligned}$$

where H denotes the Heaviside function

$$H(p) = \begin{cases} 1 & \text{if } p > 0 \\ 0 & \text{else.} \end{cases}$$

Since the derivative of the Heaviside function is the Dirac-delta-distribution, we obtain formally

$$\begin{aligned} \frac{d}{dt}J(\Omega(t)) &= \int_{\mathbb{R}^d} -H'(-\phi(x,t))\frac{\partial\phi}{\partial t}(x,t)\ g(x)\ dx \\ &= \int_{\mathbb{R}^d} \delta(\phi(x,t))|\nabla\phi(x,t)|\ V_n\ g(x)\ dx \end{aligned}$$

Now we apply the co-area formula, i.e.

$$\int_{\mathbb{R}^d} A(\phi(x))\ B(x)\ |\nabla\phi(x)|\ dx = \int_{\mathbb{R}} A(p) \int_{\{\phi=p\}} B(x)\ ds(x)\ dp.$$

This implies

$$\begin{aligned} \frac{d}{dt}J(\Omega(t))\Big|_{t=0} &= \int_{\mathbb{R}^d} \delta(\phi(x,0))\ g(x)\ V_n(x)\ |\nabla\phi(x,0)|\ dx \\ &= \int_{\mathbb{R}} \delta(p) \int_{\{\phi=p\}} g(x)\ V_n(x)\ ds\ dp \\ &= \int_{\{\phi=0\}} g(x)\ V_n(x)\ ds(x) \\ &= \int_{\partial\Omega} g\ V_n\ ds, \end{aligned}$$

i.e., we recover the above formula for the shape sensitivity.

In a similar way we can compute the shape sensitivity of the functional

$$J(\Omega) = \int_{\partial\Omega} g \; ds$$

For this sake we use again the δ-distribution and the coarea formula to deduce

$$\begin{aligned} J(\Omega(t)) &= \int_{\{\phi(.,t)=0\}} g(x) \; ds(x) \\ &= \int_{\mathbb{R}} \delta(p) \int_{\{\phi(.,t)=p\}} g(x) \; ds(x) \; dp \\ &= \int_{\mathbb{R}^d} \delta(\phi(x,t)) \; g(x) \; |\nabla\phi(x,t)| \; dx \end{aligned}$$

Thus, we can try to compute the time derivative as

$$\begin{aligned} \frac{d}{dt} J(\Omega(t)) &= \int_{\mathbb{R}^d} g \left(\delta'(\phi)|\nabla\phi|\phi_t + \delta(\phi)\frac{\nabla\phi\nabla\phi_t}{|\nabla\phi|} \right) \; dx \\ &= \int_{\mathbb{R}^d} g \left(\frac{\nabla\delta(\phi)\nabla\phi}{|\nabla\phi|}\phi_t + \delta(\phi)\frac{\nabla\phi\nabla\phi_t}{|\nabla\phi|} \right) \; dx \\ &= \int_{\mathbb{R}^d} \delta(\phi) \left(- \text{ div } \left(g\frac{\nabla\phi}{|\nabla\phi|}\phi_t \right) + g\frac{\nabla\phi\nabla\phi_t}{|\nabla\phi|} \right) \; dx \\ &= -\int_{\mathbb{R}^d} \delta(\phi) \left(\frac{\nabla g.\nabla\phi}{|\nabla\phi|}.\phi_t + g \text{ div } \left(\frac{\nabla\phi}{|\nabla\phi|} \right) \phi_t \right) \; dx \\ &= \int_{\mathbb{R}^d} \delta(\phi)|\nabla\phi| \; V_n \left(\nabla g\frac{\nabla\phi}{|\nabla\phi|} + g \text{ div } \left(\frac{\nabla\phi}{|\nabla\phi|} \right) \right) \; dx \\ &= \int_{\{\phi=0\}} V_n \left(\nabla g\frac{\nabla\phi}{|\nabla\phi|} + g \text{ div } \left(\frac{\nabla\phi}{|\nabla\phi|} \right) \right) \; ds \end{aligned}$$

One observes that on $\partial\Omega = \{\phi = 0\}$ we have

$$u = \frac{\nabla\phi}{|\nabla\phi|}, \quad \kappa = \text{ div } n = \text{ div } \left(\frac{\nabla\phi}{|\nabla\phi|} \right),$$

where n is the unit normal and κ is the mean curvature. Thus,

$$J'(\Omega)V_n = \int_\Gamma V_n \left(\frac{\partial g}{\partial n} + g \; \kappa \right) \; ds.$$

We finally notice that the above strategy of removing the term $\delta'(\phi)$ by rewriting

$$\delta'(\phi)|\nabla\phi| = \nabla\delta(\phi)\frac{\nabla\phi}{|\nabla\phi|}$$

and applying Gauss' Theorem can be used for general functionals (e.g. for second derivatives of the functional J above). In this way, we always obtain a term of the form

$$-\delta(\phi) \text{ div } \left(\frac{\nabla\phi}{|\nabla\phi|} \right),$$

i.e., the mean curvature on $\{\phi = 0\} = \partial\Omega$. In particular, we can rewrite all derivatives as surface integrals on $\partial\Omega$, involving only natural geometric quantities like the normal n or the curvature κ, its normal derivative $\frac{\partial\kappa}{\partial n}$, etc. It is a good advice to check all quantities that one obtains by computing shape sensitivities in this way with respect to their geometric meaning. If some terms do not have a geometric interpretation, then most likely the calculation was wrong.

5.2.2 Numerical Solution

In order to obtain computational methods for shape optimization problems we can again employ the level set method. In principle, we can apply any of the optimization methods discussed in chapter 4, once we know how to compute derivatives. The major difference is the way we update the design variable. In the setting of chapter 4, we have computed a search direction s to obtain

$$u_{k+1} = u_j + \tau_k s.$$

Obviously, we cannot use the same strategy in shape optimization, since a formula like

$$\Omega_{k+1} = \Omega_k + \tau_k s$$

does not make sense for shapes Ω_k. However, there is a natural update offered by the speed method. First we notice that the update for a design variable u in a Hilbert space can be rewritten as

$$u_{k+1} = u(\tau_k), \quad \frac{du}{dt} = s, \quad u(0) = u_k.$$

As in the context of shape derivatives, the corresponding speed method for shapes gives

$$\Omega_{k+1} = \left\{ x(t_k) \;\middle|\; \frac{dx}{dt} = s,\ x(0) \in \Omega_k \right\}.$$

Since the motion depends only on the normal velocity on $\partial\Omega$, we can define the update also via the level set method as

$$\begin{aligned} \Omega_{k+1} &= \{\phi(., \tau_k) < 0\} \\ \frac{\partial\phi}{\partial t} + s_n|\nabla\phi| &= 0 \quad \text{in } (0, \tau_k) \\ \{\phi(., 0\} &= \Omega_k, \end{aligned}$$

where s_n is the normal component of the update s. Hence, the iterative method is characterized by choosing a normal update. Below, we shall detail some possible ways for choosing this update.

We start with a gradient-type method. One observes that for optimization in Hilbert spaces, the gradient method is characterized by choosing the update s via

$$< s, v >= -J'(u)v \quad \forall v \in \mathcal{U}.$$

We can now write an analogous formula for the update s_n, namely

$$< s_n, V_n >= -J'(\Omega)V_n \quad \forall V_n \in \mathcal{U},$$

where $\mathcal{U}$ is a suitable Hilbert space for which we have several possibilities. We start with the simple choice $\mathcal{U} = L^2(\partial\Omega)$, i.e.,

$$< S_n, V_n >= \int_{\partial\Omega} S_n V_n \; ds.$$

As we have seen above, one can usually write the shape sensitivity in the form

$$J'(\Omega)V_n = \int_{\partial\Omega} h.V_n \; ds$$

(with $h = g$ for $J(\Omega) = \int_\Omega g \; dx$, and $h = \frac{\partial g}{\partial n} + g\kappa$ for $J(\Omega) = \int_{\partial\Omega} g \; ds$). Thus, the equation for S_n becomes

$$\begin{aligned} \int_{\partial\Omega} S_n V_n \; ds =< S_n, V_n > &= -J'(\Omega)V_n \\ &= -\int_{\partial\Omega} h \; V_n \; ds \quad \forall V_n \in L^2(\partial\Omega) \end{aligned}$$

which is equivalent to choosing $S_n = -h$.

Another interesting Hilbert space is $H^1(\partial\Omega)$. The scalar product in this space is given by

$$\begin{aligned} < S_n, V_n > &= \int_{\partial\Omega} (\nabla_s S_n \nabla_s \; V_n + S_n V_n) \; ds \\ &= \int_{\partial\Omega} V_n(-\Delta_s S_n + S_n) \; ds, \end{aligned}$$

where Δ_s denotes the gradient with respect to the surface variable S on $\partial\Omega$ and Δ_s is the surface Laplacian. Consequently, the update S_n can be computed by solving the Laplace-Beltrami equation

$$-\Delta_s S_n - S_n = h$$

on $\partial\Omega$ (note that we do not need a boundary condition, since the boundary of the surface $\partial\Omega$ is empty).

In general, we can write a Hilbert space scalar product as

$$< S_n, V_n >= \int_{\partial\Omega} (AS_n)V_n \; ds,$$

where A is a positive definite operator. Thus, we may choose any search direction of the form

$$S_n = -A^{-1}h,$$

where A is a positive definite operator. Since

$$J'(\Omega)S_n = - < S_n, S_n >= -\|S_n\|^2,$$

this yields a descent direction and we can use line search techniques to find a reasonable τ_k.

In a similar way to gradient methods we can derive Newton-type methods, for which S_n is choosen solving

$$J''(\Omega)(S_n, V_n) = -J'(\Omega)V_n, \quad \forall V_n \in \mathcal{U}.$$

5.3 Topological Derivatives

The approach that is most closely related to shape optimization uses topological derivatives as a criterion to introduce holes in addition to shape derivatives for moving shapes. The topological derivative measures the first-order variation of the objective when introducing an infinitesimal hole, usually limited to a spherical shape. I.e., the topological derivative of a functional J at topology $\Omega \subset \mathbb{R}^d$ with respect to a variation at $x \in \mathbb{R}^d$ is given by

$$d_T J(\Omega; x) = \lim_{R \downarrow 0} \frac{J(\Omega \backslash B_R(x)) - J(\Omega)}{|B_R(x)|}.$$

One observes that for $d_T J(\Omega; x) < 0$ the nucleation of a small hole centered at x is favorable, since

$$J(\Omega \backslash B_R(x)) < J(\Omega)$$

for R sufficiently small. Thus, one can combine the use of the topological derivative with shape optimization techniques, e.g. by alternating the nucleation of holes and the motion of the arising shapes.

We consider a simple example: Let

$$J(\Omega) = \int_D f(u_\Omega)\ dx,$$

where $f : \mathbb{R} \to \mathbb{R}$ is a smooth given function, and $u_\Omega \in H_0^1(\Omega)$ solves

$$-\Delta u_\Omega = \chi_\Omega \quad \text{in } D \supset\supset \Omega.$$

Then the topological derivative is given by

$$d_T J(\Omega; \overline{x}) = \int_D f'(u_\Omega) u'\ dx,$$

where

$$u' = \lim_{R \downarrow 0} \frac{u_{\Omega \backslash B_R(\overline{x})} - u_\Omega}{|B_R(\overline{x})|}.$$

Since

$$-\Delta(u_{\Omega \backslash B_R(\overline{x})} - u_\Omega) = \chi_{\Omega \backslash B_R(\overline{x})} - \chi_\Omega = -\chi_{B_R(\overline{x})}$$

we obtain

$$-\Delta u' = -\delta(\overline{x}),$$

and hence, $u' = -G(.; \overline{x})$, where G is the Green function of the Laplace operator on D.

Using topological derivatives leads to a method with clear geometric interpretation, but it suffers from two major drawbacks in general. First of all, it is difficult to switch between topological and shape derivatives in an automatic way. Secondly, the topological derivative has difficulties to handle surface functionals. Consider e.g., the case of

$$J(\Omega) = \int_\Omega g\ dx + \int_{\partial\Omega} 1\ ds.$$

Then

$$\begin{aligned} J(\Omega\backslash B_R(\overline{x})) - J(\Omega) &= \int_{B_R(\overline{x})} g \; dx + \int_{\partial B_R(\overline{x})} 1 \; ds \\ &= \int_{B_R(\overline{x})} g \; dx + 2\pi R. \end{aligned}$$

Thus,

$$\frac{J(\Omega\backslash B_R(\overline{x})) - J(\Omega)}{R^2\pi} = \frac{2\pi}{R} + \frac{\int_{B_R(\overline{x})} g \; dx}{R^2\pi} = o\left(\frac{1}{R}\right),$$

and the limit $R \to 0$ always gives $+\infty$, i.e., the topological derivative cannot generate a hole. We shall therefore consider alternative approaches in the following sections.

5.4 Phase-Field Methods

In this section we consider functionals of the form

$$\begin{aligned} J(\Omega) &= G(\chi_\Omega) + \alpha \int |\nabla \chi_\Omega| \; dx \\ &= G(\chi_\Omega) + \alpha \int_{\partial\Omega} 1 \; ds, \end{aligned}$$

where χ_Ω denotes the indicator function of the set Ω. Then one can try to approximate the minimization with respect to the signed distance function by the minimization of

$$\tilde{J}(u) = G(u) + \alpha \int_{\mathbb{R}^d} \left(\epsilon |\nabla u|^2 + \frac{1}{\epsilon} W(u) \right) \; dx$$

with respect to $u \in H_0^1(\Omega)$, where $\epsilon > 0$ is a small parameter and W is a double-well potential with minima at $u = 0, u = 1$, e.g.

$$W(u) = u^2(1-u)^2.$$

One can show that the functional $\tilde{J}$ converges to the original functional J as $\epsilon \to 0$ (in an appropriate sense).

One can interpret the ϵ-dependent terms in $\tilde{J}$ as penalizations: the term $\frac{1}{\epsilon}W(u)$ favors the values $u = 0$ and $u = 1$ and causes the convergence to indicator functions as $\epsilon \to 0$. The term $\epsilon|\nabla u|^2$ penalizes oscillations in u and causes the boundedness of the perimeter $\int |\nabla u| \; dx$ as $\epsilon \to 0$.

The phase-field method allows to use standard otpimization techniques in the Hilbert space $H_0^1(\Omega)$. Moreover, the parameter ϵ can be used to obtain a continuation strategy, i.e., one can start the optimization procedure by computing a minimizer of $\tilde{J}$ for large $\epsilon = \epsilon_1$, where the problem is globally convex, use the result as a starting value for the minimization with $\epsilon = \epsilon_2 < \epsilon_1$, and so on. In this way one can compute global minima of $\tilde{J}$, although this functional is non-convex for small ϵ in general.

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